International Conference on Spectral and High Order Methods

Herzliya, Israel
June 22-26, 1998

BOOK OF ABSTRACTS

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This is an interdisciplinary conference. Topics include theoretical, applied, and computational aspects of high order and spectral methods. Specific subjects to be addressed include spectral methods, high order finite difference and finite element methods, and wavelet-based methods for the solution of partial differential equations. Applications to be considered include electromagnetics, fluid and structural dynamics problems, efficient solvers for high order methods, and parallel aspects of spectral and high order methods.

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RECENT DEVELOPMENTS IN FINITE DIFFERENCE METHODOLOGY

ICO98-I1

By Mark Carpenter

Several topics of current interest are presented. We begin with a discussion on the relative merits of high-order shock capturing schemes. Several different discretization techniques are used to show that that all high-order schemes revert to first-order accuracy downstream of a shock, unless special provision is made to account for the shock position. Thus, it is necessary to use both H- and P-refinement in problems having discontinuous solutions. We next present a new approach to deal with complex geometries using multi-domain high-order finite-difference techniques. Special treatments at zonal boundaries guarantee stability, conservation and design accuracy between domains. Several test cases are presented that highlight the new techniques. Finally, we present some new additive (explicit/implicit) Runge-Kutta schemes that show promise in alleviating numerical stiffness in a multi-domain context.

A Survey on some Implementation Techniques of High-Order Methods in Engineering Applications

ICO98-I2

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Some twenty years ago high-order methods (spectral, collocation...) for the solution of partial differential equations seemed applicable only to peculiar classes of problems with simple geometries, regular solutions absence of numerical round-off errors, etc... In short the usefulness of these methods in engineering problems was very much put in question by their potential users. The picture has changed in the mean time, many obstacles having been removed which prevented these computation techniques to be used with maximum performance. However, the (relative) lack of interest still remains. A critical discussion of recent achievements and identification of pending problems seems therefore quite appropriate.

In the first part of this talk we review some key factors in the change: the introduction of preconditioning techniques, the treatment of deformed geometries, time integration algorithms, etc... In a second part we deal with potential future developments, in particular related to the emergence of new programming paradigms (C++, Java) and computer architectures.

Detection of Edges in Spectral Data

Eitan Tadmor

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ICOSAHOM '98

ABSTRACT

We address the fundamental problem of detecting the edges of piecewise smooth data from its given spectral content. We introduce a novel method to detect such edges, based on the use of appropriate *concentration factors*, $\sigma(\frac{k}{N})$.

Specifically, let the Fourier coefficients be given, $\{\hat{f}_k\}_{k=-N}^{N}$. To detect the edges of the underlying piecewise smooth $f(\cdot)$, one employs an admissible concentration function $\sigma(\cdot)$ — an odd function which satisfies $\int_{\frac{1}{N}}^{1} \frac{\sigma(x)}{x} dx \to -\pi$. It is shown that for all admissible σ's, the corresponding generalized conjugate partial sum, $\tilde{S}_N^{\sigma}[f](x) := i \sum_{k=-N}^{N} \sigma(\frac{k}{N}) \hat{f}_k e^{ikx}$, converges to the jump function $[f](x) := f(x+) - f(x-)$. Thus, $\tilde{S}_N^{\sigma}[f]$ vanishes in smooth regions of f and it tends to 'concentrate' near the edges of f.

We demonstrate the examples of two families of admissible concentration factors: the Fourier factors, $\sigma_{\alpha}^{F}(x) = \frac{-\pi}{Si(\alpha)} \sin \alpha x$, and the polynomial factors, $\sigma^{p}(x) = -p\pi x^{p}$. These yield effective detectors of one or more edges, where both the location and the amplitude of the discontinuities are recovered.

We then proceed to describe a novel *enhancement* procedure based on enhancement of the different scales separating the smooth pieces from their defining edges. The enhancement procedure is (1) *nonlinear*; (2) *simple to implement*; and (3) *remarkably effective*.

Numerical experiments, with both periodic and non-periodic data, demonstrate how the use of concentration factors coupled with a simple enhancement procedure enables one to *pinpoint* the location of the underlying edges within the given spectral data.

NUMERICAL ANALYSIS OF SINGULARITIES ASSOCIATED WITH ELLIPTIC PROBLEMS BY P-FEM

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In many important linear elliptic problems, e.g. elasticity or heat transfer, the exact solution has one or more singular points (or edges in 3-D). These may be caused by an abrupt change in the boundary geometry, abrupt changes in boundary conditions or material properties. In the vicinity of the singular points the solution is typically characterized by a sequence of eigenpairs. The determination of these eigenpairs, and reliable computation of the coefficients of the asymptotic expansion, are of great practical importance because failure theories directly or indirectly involve these coefficients. Examples encountered in engineering practice are provided.

New methods for the computation of eigenpairs and the determination of the coefficients of the asymptotic expansion for singularities associated with corners and edges, multi-material interfaces and abrupt changes in boundary conditions will be presented for 2-D as well as 3-D domains [1, 2, 3, 4]. The methods are based on the modified Steklov weak formulation and the principle of complementary energy in conjunction with the p-version of the finite element method. Superconvergent rates of the computed data is demonstrated.

An extension of above methods for non-homogeneous elliptic problems, as thermo-elasticity, will be also addressed [5].

Numerical examples for 2-D and 3-D elastostatic problems, including singularities associated with multi-material interfaces and anisotropic domains as well as 2-D thermo-elastic singular problems are provided to demonstrate the efficiency and accuracy of the proposed approach when used in conjunction with the p-version of the finite element method.

References

[1] Szabó, B. A. and Yosibash, Z. Superconvergent computations of flux intensity factors and first derivatives by the FEM. *Comp. Meth. Appl. Mech. Engrg.*.. 129, (1997), pp. 349-370.

[2] YOSIBASH, Z. AND SZABÓ, B. A. Numerical analysis of singularities in two-dimensions. Part 1: Computation of eigenpairs. *Int. Jour. Numer. Meth. Engrg.*, **38**, (1995), pp. 2055-2082.

[3] SZABÓ, B. A. AND YOSIBASH, Z. Numerical analysis of singularities in two-dimensions. Part 2: Computation of the generalized flux/stress intensity factors. *Int. Jour. Numer. Meth. Engrg.*, **39**, (1996), pp. 409-434.

[4] Z. YOSIBASH. Numerical analysis of edge singularities in three-dimensional elasticity. *Int. Jour. Numer. Meth. Engrg.*, **40**, (1997), pp. 4611-4632.

[5] Z. YOSIBASH. Numerical thermo-elastic analysis of singularities in two-dimensions. *Int. Jour. Fracture*, **74**, (1996), pp. 341-361.

Spectral Penalty Methods

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One of the central problems in developing and analyzing high-order methods, and in particular spectral methods, for the solution of partial differential equations results from the need to impose boundary conditions. In the traditional approach boundary conditions are enforced strongly by directly modifying the operators, be they spectral space operators or pseudospectral differentiation matrices, hence ruining the very delicate structure of the operators. Moreover, this approach is wellknown to be increasingly complicated for complex boundary operators and it significantly complicates the analysis of the complete schemes.

A technique for overcoming some, if not all, of the aforementioned problems is offered by the spectral penalty methods. This approach involves enforcing the boundary conditions in a weak way only, although at an accuracy of the order of the scheme, hence without loss of the overall spectral accuracy.

In this talk we shall review the development and formulation of the spectral penalty methods. As we shall see through a number of examples, this approach alleviates many of the above problems and provides a constructive approach for the development of asymptotic stable schemes for the solutions of partial differential equations. Moreover, it removes many of the theoretical problems traditionally associated with the analysis of spectral methods as a result of the operators and the boundary conditions being dealt with in a separate manner.

To illustrate the analysis as well as the versatility of the penalty methods we shall discuss the construction of stable schemes for problems with non-trivial boundary conditions, the formulation of very efficient preconditioners for pseudospectral operators and the development of stable spectral schemes for the solution of partial differential equations on generally unstructured grids in two and three dimensions. We will conclude the talk with drawing a few parallels between penalty methods and recent developments in high-order finite difference and finite element methods.

ICO98-I6

Domain Decomposition Methods for Higher Order Finite Element Methods

Olof B. Widlund

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Domain decomposition methods have been developed quite systematically and successfully in particular for conforming, lower order finite element approximations of elliptic problems. These algorithms are preconditioned conjugate gradient-type methods based on solvers for subregions and certain low-dimensional global models. The best results show that the convergence rate is independent of the number of local subproblems, which form an important part of the preconditioner, and depends only polylogarithmically on the size of the local problems.

The basic domain decomposition methods were extended to spectral elements and scalar elliptic problems in series of papers written jointly with Luca Pavarino about four years ago. In this talk, our more recent work on elliptic systems and mixed methods will be discussed. An account will also be given of results obtained by Ion Bica, in a recent Courant Institute doctoral dissertation, for p-version finite element methods.

A Fully Fourth-Order Accurate Finite Volume Method For Steady and Transient Flow Problems

by

C.B. da Silva, J.M.M. Sousa and J.C.F. Pereira*

A fully fourth-order accurate finite volume method for the solution of steady and transient incompressible Navier-Stokes flows using a collocated arrangement of primitive variables is presented. The talk is focused on two related issues arising in the discretization of the expressions resulting from the application of Gauss' theorem to the governing equations. The first concerns the integration procedure to evaluate the fluxes at control volume faces. The second regards fourth-order consistency between the finite difference counterpart of gradient and divergence operators arising in pressure (Poisson) and momentum equations using the pressure-weighted interpolation method [1].

A straight-forward procedure to achieve higher-order accuracy in the approximation of the derivatives appearing in the equations governing flow motion is to employ Lagrange interpolating polynomials [2]. This approach is particularly flexible, presenting the additional advantage of allowing the use of non-uniform grids without loss of generality. In finite volume methods, high-order interpolation using the polynomials and their derivatives may be applied when calculating convection and diffusion fluxes at control volume faces [3]. Nevertheless, the approximation of surface and volume integrals in the control volume is, as a general precept, constructed by using the midpoint rule [3, 4]. Thus, as the numerical grid is successively refined, the resulting numerical scheme exhibits an asymptotic convergence corresponding to second-order accuracy, irrespectively of higher-order interpolation [5]. In order to retain fourth-order consistency in the numerical method, both interpolations and integrations must be calculated with compatible accuracy. The present method makes use of a 3-point Simpson's rule to approximate surface integrals, while 9 points are employed to compute volume integrals (two-dimensional case). As an example, this translates into an actual 15-node dependency for all cell fluxes. It should be furthermore noted that this issue only arises when considering a finite volume formulation. Although a non-conservative formulation should perform as well as the conservative counterpart in the absence of flow discontinuities, high-order accurate methods subjected to the constraint of global conservation of fluxes are highly desirable [6].

Another advantageous feature of the present finite volume method is the collocated arrangement of variables, which facilitates the extension to non-orthogonal grids and the numerical treatment of boundaries. However, a standard pressure-velocity coupling methodology for the calculation of incompressible fluid flow [3, 4] originates the decoupling of those quantities when the foregoing arrangement of variables is chosen. A well-known technique to avoid this difficulty is to correct the fluxes at cell faces using the pressure-weighted interpolation proposed by Rhie and Chow [1]. Yet, it must be emphasized that fourth-order consistency must be retained in this procedure as well.

In order to tackle both steady and transient problems, time integration must be performed as well. In the present method we have resorted to Runge-Kutta methods. Aiming to achieve fourth-order accuracy in time also, a four-stage algorithm has been implemented.

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In this talk we present two test cases purporting to evaluate the accuracy of the method. In the first test case, calculations of a steady regime of the unit cavity problem have been performed. Grid-convergence results were obtained in terms of L_2 norm at $Re = 1000$, unequivocally displaying the consequences of disregarding the order of approximation in numerical integrations. The "exact" solution used to estimate grid-convergence rates was computed by Richardson extrapolation from fourth-order accurate solutions. Field variables were compared with a reference solution published in the literature [7]. However, as the numerical method used in [7] to produce those results was reported to be only second-order accurate, another set of reference results of the same problem was obtained employing a multi-domain pseudo-spectral method (discretization by Chebyshev polynomials on Gauss-Lobatto points). The comparison has reinforced the above conclusions. Present results are superior to that reported in [8] employing 41 x 41 mesh points. The second test case consists in the simulation of an unsteady regime of the regularized unit cavity at $Re = 10{,}500$. In this case, reference solutions have been obtained from the spectral calculations reported in [9]. The expected time-periodic behavior could be captured by the present high-order finite volume method.

References:

[1] C.M. Rhie and W.L. Chow, *A numerical study of the turbulent flow past an isolated airfoil with trailing edge separation*, AIAA J., **21** (1983), pp. 1525-1532.

[2] J.M. Hyman and B. Larrouturou, *The numerical differentiation of discrete functions using polynomial interpolation methods*, Appl. Math. and Comp., **10-11** (1982), pp. 487-506.

[3] J.M.M. Sousa, C.F.N.B. Silva and J.C.F. Pereira, *Accuracy comparison of high-order finite difference schemes for the evolution of two-dimensional finite-amplitude disturbances*. Proc. of the Third Int. Conf. on Spectral and High Order Methods (1996), pp. 389-396.

[4] J.C.F. Pereira and J.M.M. Sousa, *Finite volume calculations of self-sustained oscillations in a grooved channel*, J. Comput. Phys., **106** (1993), pp. 19-29.

[5] Z. Lilek and M. Peric, *A fourth-order finite volume method with colocated variable arrangement*, Computers Fluids, **24** (1995), pp. 239-252.

[6] M.M. Rai and P. Moin, *Direct simulations of turbulent flow using finite-difference schemes*, J. Comput. Phys., **96** (1991), pp. 15-53.

[7] U. Ghia, K.N. Ghia and C.T. Shin, *High-Re solutions for incompressible flow using the Navier-Stokes equations and a multigrid method*, J. Comput. Phys., **48** (1982), pp. 387-411.

[8] W.F. Spotz and G.F. Carey, *High-order compact finite difference methods*. Proc. of the Third Int. Conf. on Spectral and High Order Methods (1996), pp. 397-407.

[9] J. Shen, *Hopf bifurcation of the unsteady regularized driven cavity flow*, J. Comput. Phys., **95** (1991), pp. 228-245.

A 2° ORDER FINITE VOLUME PROJECTION METHOD FOR INCOMPRESSIBLE FLUID FLOW ON UNSTRUCTURED/HYBRID GRIDS

ICO98-2

by

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ABSTRACT

A Finite-Volume method for the solution of the Navier-stokes equations for incompressible fluid flow in two dimensional arbitrary geometries is presented. The computational domain was divided into polygon triangles and quadrilaterals allowing the general use of hybrid structured/unstructured grids. In addition a new convection discretization second order Upwind Least Squares Scheme (ULSS) is proposed in the framework of primitive variables where a projection method is used to calculate the pressure field. The system of algebraic equations is solved by biconjugate gradient stabilized method (BI-CGSTAB).

The ULSS proposed in this work is based on pointwise reconstruction of the variable ϕ by a piecewise polynomial and it is required to be consistent with averaging and of high order of accuracy.

We start with the average values of ϕ stored at the centroids of the control volumes. Then, given a set τ we approximate the function ϕ over τ by either an affine or a bilinear function, depending on whether τ is a triangle or a quadrilateral, respectively. And require of this polynomial to be the least square approximation of the average values of the function at an appropriate set of neighboring points.

For the pressure velocity coupling we use a projection method and we define V as the linear space of vector fields with support at the centroid of the mesh and let S the linear space of scalar fields with support at the vertices of the mesh control volumes.

Over these spaces, we then define the gradient operator $G: S \to V$ as follows:

$$G\phi = \sum_{i \in \Omega_c} \sum_{j=1}^{d} (G\phi)_j(i) e_j(i)$$

for all $\phi \in S$, where,

$$(G\phi)_j(i) \equiv \frac{1}{m_v(\tau(i))} \sum_{f \in \partial\tau(i)} \phi_f m_s(f) n_j(f) \in R$$

for all $i \in \Omega_c$ and $j = 1, ..., d$, where $\tau(i)$ is the control volume associated with the centroid i,

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$\partial\tau(i)$ denotes its boundary, i.e., $\partial\tau(i)=\{f_1,\ldots,f_{\#f(i)}\}$, $\#f(i)$ is the number of cell faces associated with the control volume $\tau(i)$, $i\in\Omega_c$, ϕ_f is the arithmetic mean of the values of the functions ϕ_k at the vertices associated with the cell face f, and $n_j(f)$ is j-th component of the unitary exterior normal vector at cell face f, $j = 1, \ldots, d$. We similarly define the divergence operator $D:V \to S$ as follows:

$$Du=\sum_{i\in\Omega_c}\sum_{j=1}^{d}(Du)_j(i)\xi(i)$$

for all $u\in V$ where,

$$(Du)_j(i)\equiv\frac{1}{m_v(\tau^*(i))}\sum_{f\in\partial\tau^*(i)}u_f.n_f m_s(f)\in R$$

for all $i\in\Omega_v$, where $\tau^*(i)$ stands for the dual control volume associated with the vertice i, and so on.

So, with the above definitions in the projection method we proceed with a fractional time evolution given by the solution of the following linear problem FS:

Find $u^{n+1,0}\in V$ such that

$$\frac{u^{n+1,0}-u^n}{\Delta t}+D\left(Vu^n\otimes Cu^{n+1,0}-\sigma_v\left(u^{n+1,0}\right)\right)=-Gp^n$$

and

$$u^{n+1,0}_{|\partial\Omega}=g_{t^{n+1}}$$

where $g_t:\partial\Omega\to\partial\Omega\times R^d$ at each time t is a given vector field over the domain boundary $\partial\Omega$, u is the velocity vector field, p is the pressure field, Δt is the time step, σ_v is the deviation stress tensor, $\otimes$ denotes de tensor product and the super-script n denotes the value of the object at the n-th time step.

We complete the time evolution with the projection of the resulting velocity vector field $u^{n+1,0}$ into the space of solenoidal vector fields:

$$u^{n+1}=P_o\left(u^{n+1,0}-v_d\right)+v_d$$

(where v_d, is a divergenge free vector field wich vanishes on the boundary) and the computation of the pressure field from the second fractional step:

$$\frac{u^{n+1}-u^n}{\Delta t}+D\left(u^n\otimes u^{n+1,0}-\sigma_v\left(u^{n+1,0}\right)\right)=-Gp^{n+1}$$

Numerical solutions are compared with analytical solutions of a 2D test case and for driven cavity flow. The evolution of the error norm slope as a function of the mesh parameters, confirm that the proposed numerical method is second order accurate to solve 2D Navier-Stokes equations in hybrid structured/unstructured grids.

Numerical simulation for semiconductors devices using high-order compact scheme on nonuniform grid

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This work describes fourth-order compact schemes utilized to solve the coupled system of nonlinear partial differential equations which model semiconductors devices. For the sake of clarity, we restrict our attention to the bidimensional steady-state equations. We consider equations in dimensionless form given in [1] for the dependent variables (ψ, n, p) on a bounded domain Ω in R^2

$$(DD)\begin{cases} \lambda^2\Delta\psi - n + p + C(x,y) = 0, & (x,y)\in\Omega \quad \text{Poisson's equation,} \\ \text{div } Jn = \ GR(x,y), & (x,y)\in\Omega \quad \text{electron continuity equation,} \\ \text{div } Jp = -GR(x,y), & (x,y)\in\Omega \quad \text{hole continuity equation.} \end{cases}$$

ψ, n, p represent the electrostatic potential, the electron density, the hole density respectively and Jn, Jp are the current densities in the drift-diffusion form given by

$$\begin{cases} Jn = -D_n\nabla n + \mu_n n\nabla\psi, & Jn = (Jnx, Jny), \\ Jp = \ \ D_p\nabla p + \mu_p p\nabla\psi, & Jp = (Jpx, Jpy). \end{cases}$$

ψ, n, p verify the mixed Neumann and Dirichlet boundary conditions given by

$$\begin{cases} \dfrac{\partial\psi}{\partial\nu} = Jn.\nu = Jp.\nu = 0, & \text{on } \Gamma_N, \\ \psi = \psi_D, n = n_D, p = p_D, & \text{on } \Gamma_D, \end{cases}$$

where ν represents the unit outgoing vector of the domain. μ_n, μ_p, D_n, D_p are the mobility and diffusivity coefficients respectively, $C(x,y)$ is the doping profile, and $GR(x,y)$ is the generation-recombination rate. ¿From a numerical point of view, difficulties arise in discretization of advection-dominated current equations (due to the large size of $\nabla\psi$ in a significiant part of the domain). The ability to accurately compute the currents is of major importance, and the discretization of the continuity equations (requiring the determination of the currents) must be done in conservation form. The most popular and effective methods are based on the Scharfetter-Gummel method [2].

In the first part of our work, we formulate the system (DD) on staggered grid and present an alternative method using fourth-order compact difference scheme to compute current densities (preserving the conservativity) on the mid-point of mesh lines connecting neighbor grid nodes. In our case, no boundary layers occur at ohmic contacts and insulating segments, but there exist strong variations of the solutions in some regions of the device (nearby interfaces and junctions). Thus a strongly non uniform mesh is mandatory. So we present the extension of our discretization for a nonuniform grid. The derivation of an efficient scheme on a nonuniform grid is based on mapping techniques which have been previously utilized in particular for convection-diffusion problems by Spotz and Carey [3]. For a given class of discretization (control of the refinement regions), we present a simple and efficient construction of the mapping functions $x = x(\zeta, \eta)$ and $y = y(\zeta, \eta)$ based on interpolation spline, which do not introduce numerical error in the resulting scheme. Such a formulation presents the advantage to suppress artificial oscillations and yield more accurate solutions than classical methods. The transformation of the equations (DD) to a computational domain $\hat{\Omega}$ via (x, y) combined with the construction of high-order schemes requires very intricated algebraic manipulations. To overcome these difficulties, we use a symbolic computer system AXIOM which computes and generates FORTRAN codes necessary to obtain numerical results.

References

[1] - W. V. Van Roosbroeck, *Theory of flow electrons and holes in Germanium and other semiconductors.* Bell Syst. Tech. J. 29. pp. 650-607, 1950.

[2] - D.L. Scharfetter and H.K. Gummel, *Large Signal of a silicon Read Diode oscillator.* IEEE Transaction on Electron Devices, vol. ED-16, pp. 64-77, 1969.

[3] - W.F. Spotz and G.F. Carey, *Formulation and experiments with High-Order Schemes for Nonuniform Grids.* Accepted for publication. The International Journal of Numerical Methods for Heat & Fluid Flow, April 1997.

Stable High–Order Finite Difference Methods for the compressible Navier–Stokes equations

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We derived stability results for high–order finite difference approximations to the compressible Navier–Stokes equations on bounded curvi–linear domains. The main tools used in the derivation of the stability estimate are a change of variables that symmetrizes the equations, a special splitting of the advective (Euler) fluxes and summation–by–parts.

High-Order, Finite Differences, Stability 65M12

1 Introduction

In the last five years, stable high–order finite difference schemes were derived for a large class of linear initial boundary value problems [8, 9, 10]. In [7] it was shown how to treat nonlinear conservation laws and recently in [1] a stable high–order finite difference scheme was designed for the Euler equations of gasdynamics on curvilinear bounded domains (the one–dimensional results were presented by the authors at the ICOSAHOM conference in 1995). The Euler scheme has been tested numerically and was shown to be robust and efficient [3]. The scheme is implemented in a software package for composite adaptive grid methods (SIMCOP). The main criteria in developing SIMCOP are efficiency and simplicity. We are now in the process of extending SIMCOP to include the compressible Navier–Stokes equations. In this paper we describe how to derive stability estimates for the two–dimensional Navier–Stokes equations in cartesian coordinates. The results can be

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extended in a straightforward way to three space dimensions. General curvilinear coordinates can be dealt with using the same approach as in [1].

2 The two–dimensional Navier–Stokes equations

We write the compressible Navier–Stokes equations as

$$u_{,t} + f_{i,i} = f^v_{i,i} + f^h_{i,i} = (K_{ij}u_{,j})_{,i} \tag{1}$$

where $f^v_i = K_{ij}u_{,j}$, $f^h_i = K^h_{ij}u_{,j}$, $K_{ij} = K^v_{ij} + K^h_{ij}$,[1] and

$$\begin{aligned}
u &= (\ \rho & \rho u & & \rho v & & E\ )^T \\
f_i &= (\ \rho u_i & \rho u_1 u_i + p\delta_{i1} & & \rho u_2 u_i + p\delta_{i2} & & u_i(E+p)\ )^T \\
f^v_i &= (\ 0 & \tau_{1i} & & \tau_{2i} & & u_j\tau_{ij}\ )^T \\
f^h_i &= (\ 0 & 0 & & 0 & & -kT_{,i}\ )^T
\end{aligned}$$

The variable ρ is the density, u_i is the velocity in the x_i–direction, E is the total energy, T the temperature and p the pressure. The vectors f_i are the Euler fluxes, f^v_i are the viscous fluxes and f^h_i are the heat fluxes. The constant k is the heat conductivity. We use the constitutive equations $p = (\gamma-1)(E - \frac{1}{2}\rho(u_1^2+u_2^2))$, $\tau_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i})$, where γ is the ratio of specific heats and λ and μ are the viscosity coefficients. The non–dimensionalized entropy S is given by $S = \log p\rho^{-\gamma}$. The boundary conditions are as suggested in lemma 7.7.1 in [6] to ensure well–posedness.

3 Stability estimates

The semi–discrete stability estimates are derived using the energy method. The principal tool that enables the derivation of these energy estimates is summation–by–parts, a discrete analogue of integration–by–parts used in the continuous energy method. Discretization operators that satisfy the summation–by–parts property are presented in [11]. In principle, we follow the same steps as in the derivation of the stable scheme for the Euler equations [3]:

1. *Symmetrize the fluxes using a change to so–called entropy variables* $w = w(u)$ *[4].* The entropy variables are given by $w(u) = \eta_{,u}$. The scalar function

[1] In the index notation $\cdot_{,j} \equiv \frac{\partial \cdot}{\partial x_j}$. The summation convention holds.

$\eta(u) = -\rho h(S)$ is convex and $h(S)$ is an arbitrary but differentiable function of the entropy S. The transformed system is

$$u_{,t} + \tilde{f}_{i,i} = (\tilde{K}_{ij} w_{,j})_{,i}, \tag{2}$$

with $\tilde{f}_{i,w}^T = \tilde{f}_{i,w}$. We use the tilde-notation to indicate that the terms are now written as functions of w. For the Euler equations it was convenient to use a transformation that preserved the homogeneity property of the Euler fluxes, i.e. $f_i(\beta u) = \beta f_i(u)$. This simplified the treatment of the characteristic boundary conditions. Because of the different nature of the boundary conditions for the Navier–Stokes equations homogeneity is no longer needed. Instead we choose η such that $\tilde{K}$, defined by

$$\tilde{K} = \begin{pmatrix} \tilde{K}_{11} & \tilde{K}_{12} \\ \tilde{K}_{21} & \tilde{K}_{22} \end{pmatrix},$$

is symmetric and positive definite. This is possible for $\eta = -\rho S$, as shown in [5]. This gives

$$w = \frac{(\gamma - 1)}{p}\Big(-E + \frac{p}{\gamma - 1}(\gamma + 1 - S) \quad \rho u_1 \quad \rho u_2 \quad \rho\Big)^T$$

Expressions for the flux vectors and diffusion matrices are given in [5].

2. *Apply the canonical splitting to the symmetrized Euler fluxes.* Following the approach in [7, 3] we construct vector functions F_i such that $F_{i,w} w = -F_i + \tilde{f}_i$. This gives

$$\tilde{f}_{i,i} = (F_{i,w} w)_{,i} + F_{i,i}.$$

Equation (2) can now be written as

$$u_{,t} = -(F_{i,w} w)_{,i} - F_{i,i} + (\tilde{K}_{ij} w_{,j})_{,i}. \tag{3}$$

3. *Discretize (3) in space using the discretization operators D_i for the x_i-direction that satisfy the summation-by-parts property [8].* At the boundary, the discretization operators are one-sided and of order $r, r \geq 1$. In the interior, they are of order $2r$. We get

$$u_{,t} = R(w) = -D_i(F_{i,w} w + F_i) + D_i(\tilde{K}_{ij} D_j w). \tag{4}$$

4. *Construct a projection operator P that forces the solution to satisfy the analytic boundary conditions.* We write the boundary conditions as $L^T w = b$,

where $b = b(x, y, t)$ and L is a constant matrix with full rank. The projection operator is constructed as

$$P = I - L(L^T w_u L^{-1})^{-1} L^T w_u.$$

Following a similar approach as in [1] it can be shown that the semi-discrete solution $u(w)$ satisfies

$$u_{,t} = PR(w), \tag{5}$$

provided the boundary and initial data satisfy suitable compatibility criteria.

5. *Take the scalar product of (5) with w and apply summation-by-parts.* The final estimate can be written in the form

$$\|w\|_U^2 \leq \|h\|_U^2 + K \int_0^t \|b\|_\Gamma d\tau, \tag{6}$$

where h are the initial data and K is a constant. The subscript U indicates that the scalar norm is weighted by the matrix U, which is positive definite. The subscript Γ indicates that the norm is computed at the boundary. We remark that $\|w\|_U^2$ is a discrete entropy function and that (6) can be interpreted as an entropy inequality.

References

[1] M. Gerritsen, *Designing an efficient solution strategy for fluid flows*, PhD thesis, Stanford University (1996).

[2] M. Gerritsen and P. Olsson, *Designing an Efficient Solution Strategy for Fluid Flows: I. A High-Order Stable Finite Difference Scheme and Sharp Shock Resolution*, J. Comput. Phys., 129 (1996).

[3] M. Gerritsen and P. Olsson, *Designing an Efficient Solution Strategy for Fluid Flows: II. Stable high-order central finite difference schemes on composite adaptive grids with sharp shock resolution*, submitted J. Comput. Phys. (1997).

[4] A. Harten, *On the symmetric form of systems of conservation laws with entropy*, J. Comput. Phys., 49 (1983), pp. 151–164.

[5] T. J. R Hughes, L. P. Franca and M. Mallat, *A new finite element formulation for computational fluid dynamics: I. Symmetric forms of the compressible Euler and Navier–Stokes equations and the second law of thermodynamics* Comput. Meth. Appl. Mech. Eng., 54 (1986)

[6] H.-O. Kreiss and J. Lorenz, *Initial–Boundary value problems and the Navier–Stokes equations*, Pure and Applied Mathematics, 136 (1989)

[7] P. Olsson, *Energy and maximum norm estimates for nonlinear conservation laws*, RIACS 94-01 (1994)

[8] P. Olsson, *Summation by parts, projections, and stability I*, Math. Comp., 64 (1995), pp. 1035–1065.

[9] P. Olsson, *Summation by Parts, Projections and Stability II*, Math. Comp.64 (1995), pp. 1473–1493.

[10] P. Olsson, *Summation by Parts, Projections and Stability III*, RIACS 95-06 (1995).

[11] B. Strand, *Summation by parts for finite difference approximations for d/dx*, J. Comput. Phys., 110(1) (1994), pp. 47–67.

Stability properties of boundary- and interface treatment in spectral methods for hyperbolic problems

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Motivated by simulation of internal gravity waves in the ocean, we study a system of partial differential equations on the form

$$\frac{\partial \mathbf{u}}{\partial t} + \sum_{i=1}^{3} A_i \frac{\partial \mathbf{u}}{\partial x_i} = \sum_{|\alpha|=2} B_\alpha \frac{\partial^\alpha \mathbf{u}}{\partial \mathbf{x}^\alpha} + \mathbf{f}, \tag{1}$$

where $\mathbf{u}(\mathbf{x}, t)$ and $\mathbf{f}$ are in $\mathbf{R}^m$, each A_i and B_α are $(m \times m)$-matrices, and α is a multi-index. This is solved through a semi-implicit splitting method, with the three steps

$$\frac{\partial \mathbf{u}^I}{\partial t} + \sum_{i=1}^{3} P_i^I \frac{\partial \mathbf{u}^I}{\partial x_i} = \mathbf{f}^I, \tag{2}$$

$$\frac{\partial \mathbf{u}^{II}}{\partial t} + \sum_{i=1}^{3} P_i^{II} \frac{\partial \mathbf{u}^{II}}{\partial x_i} = \mathbf{f}^{II}, \tag{3}$$

$$\frac{\partial \mathbf{u}^{III}}{\partial t} = \sum_{|\alpha|=2} P_\alpha^{III} \frac{\partial^\alpha \mathbf{u}^{III}}{\partial \mathbf{x}^\alpha}. \tag{4}$$

The first step (2) is a hyperbolic system, and is advanced one time-step by explicit time-integration. The second and third steps (3), (4) are discretized by the Crank-Nicolson method and solved implicitly through reduction to Helmholtz equations [1].

We focus on the first step here, and present a systematic study of different formulations of boundary conditions for hyperbolic problems with respect to the stability properties of explicit time-integration. For the use of domain decomposition methods, we also consider subdomain interface conditions.

Boundary- and interface conditions can either be incorporated in the semi-discretization of the problem and solved as ordinary differential equations, or implemented as corrections after each time-step. In the first category we consider ODE-formulation based on integrating the compatibility conditions [2, 3], and the penalty method where a combination of the PDE and the boundary- or interface conditions is integrated [4].

The classical correction method based on characteristics [5, 6] is included, as well as correction based on continuity of derivatives. The latter method is motivated by the splitting method described above, because the second and third steps will also influence the stability properties

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of the full system. Preliminary results indicate that the stability of the full method improves with the smoothness across interfaces of the intermediate solution from the first step.

For each of the methods, propagation matrices of full discretizations using explicit time-integration are constructed for the advection equation in one and two dimensions, and analysed in terms of eigenvalues and pseudoeigenvalues [7]. The matrices involved are not normal, but the numerical results indicate that the essential information for stability can still be found in the eigenvalues.

We explore the differences between one- and two-dimensional problems in a single domain as well as in a multidomain setting. For the interfaces (not including corners) in two-dimensional problems we may use conditions based on the one-dimensional approach or use conditions involving tangential derivatives. We present results with the former approach. Corner points have to be given special consideration, and there is no canonical way of treating corner points for hyperbolic systems. We present and discuss results for two corner point strategies having different stability limits.

To illustrate the applicability of the different methods in more realistic examples than simple model problems, we also look at systems of equations in two dimensions, with automatic time-step control as indicator of the stability properties.

References

[1] M. Bjørhus. A semi-implicit method for compressible isenthropic ocean dynamics. Part I: General formulation. Technical Report FFI/RAPPORT-97/02045, Norwegian Defence Research Establishment, P.O. Box 25, N-2007 Kjeller, Norway, May 1997.

[2] A. Quarteroni. Domain decomposition methods for systems of conservation laws: Spectral collocation approximations. *SIAM J. Sci. Stat. Comput.*, 11:1029–1052, 1990.

[3] M. Bjørhus. The ODE formulation of hyperbolic PDEs discretized by the spectral collocation method. *SIAM J. Sci. Comput.*, 16:542–558, 1995.

[4] D. Funaro and D. Gottlieb. A new method of imposing boundary conditions in pseudospectral approximations of hyperbolic equations. *Math. Comp.*, 51:599–611, 1988.

[5] D. Gottlieb, M. Gunzburger, and E. Turkel. On numerical boundary treatment of hyperbolic systems for finite difference and finite element methods. *SIAM J. Numer. Anal.*, 19:671–682, 1982.

[6] D. A. Kopriva. Multidomain spectral solution of the Euler gas-dynamics equations. *J. Comput. Phys.*, 96:428–450, 1991.

[7] S. C. Reddy and L. N. Trefethen. Stability of the method of lines. *Numer. Math.*, 62:235–267, 1992.

An efficient spectral iterative domain decomposition technique for the incompressible Navier-Stokes Equations

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ABSTRACT

The main objective of this study is to provide an efficient tool for the extension of spectral methods to complex geometries, tall cavities, or in the presence of discontinuities, while preserving their computational efficiency and their high order accuracy. A significant motivation for the use of spectral approximations stems for their very low phase errors for the prediction of time-dependent flows, besides their high resolution [1]-[2]. Partitioning (which can be also combined with mapping technique) has proven now to be an efficient tool to allow the use of spectral approximations to more general geometries, particularly to treat the presence of any discontinuity inside the domain. A comprehensive review of such approaches can be found in Canuto et al. [2]. Three main families of domain decomposition technique have been identified by these authors: the patching methods, the alternating Schwarz methods or overlapping methods, and the variational or spectral element methods. The present study concerns the first ones, using the patching-collocation method suggested by Orszag [3]. The development is specially oriented to the parallel computing implementation.

The domain decomposition requires to ensure the continuity of variables and their normal gradient between two adjacent subdomains for the resolution of the Navier-Stokes equations. Direct coupled methods have been proposed in literature to treat these conditions as the influence matrix technique ([4]). This was done successfully for two-dimensional and axisymmetric flows using the vorticity-streamfunction formulation [5]. However, its extension to three-dimensional flows, which corresponds also to our final goal, is difficult to manage. Moreover, its application to primitive variables has shown limitations to satisfy the continuity of normal pressure derivative at interface, due to the Neumann boundary conditions. Zanolli [6] has proposed a suitable iterative procedure to ensure these continuities. For linear problems having Dirichlet or mixed boundary conditions (BCs), the method consists in solving alternately Dirichlet and Neuman BCs at interfaces between adjacent subdomains by introducing a relaxation parameter. Funaro et al. [7] have provided a rigourous convergence analysis of the algorithm, and proved that under some circumstances, an optimal value of the relaxation parameter can be obtained to achieve the convergence in small number of internal iterations (2 or 3). These authors have also proposed an effective dynamical choice of the relaxation par-

The present study corresponds to an extension of this iterative technique for the resolution of the incompressible Navier-Stokes equations. In view of solving the indetermination induced by the Neumann BCs for the pressure Poisson equation, the same type of BCs has been imposed successively at interfaces, resulting from previous time step. The continuity of variables is first satisfied through the relaxation parameter, followed by Neumann condition for the normal derivatives. Moreover, it allows a more efficient parallel computing, by eliminating the synchronization problem encountered in the previous form. In each subdomain, the numerical approach is based on Chebyshev-collocation method associated with a stiffly stable second order time scheme. The coupling of the velocity and the pressure is treated by using an efficient projection scheme, which ensures a divergence free velocity field at each iteration ([8]). Complete diagonalization of operators reduces the resolution to simple matrices products at each time step.

First applications concern the prediction of different bifurcations and transitions of flow regimes occurring in tall differentially heated cavity. Indeed, the use of domain decomposition in tall cavities does improve the conditioning of the algebraic problem by reducing the ratio of largest to smallest grid spacing. The purpose is to delineate a stability diagram, which can complete theoretical studies in such configuration for a low Prandtl number fluid (Pr=0.01).

References

[1] Gottlieb D. and Orszag S.A., *Numerical analysis of spectral methods: Theory and Applications.* CBMS Regional Conf. Series in Appl. Math., SIAM, 1977.

[2] Canuto C., Hussaini M.Y., Quarteroni A. and Zang T.A., *Spectral methods in fluid dynamics.* Springer Verlag, 1987.

[3] Orszag S. A., 'Spectral methods for problem in complex geometries', *J. Comp. Phys.*, **37**, 70-92, 1980.

[4] Raspo I., Ouazzani J. and Peyret R., 'A spectral multidomain technique for the computation of the Czochralski melt configuration', *Int. J. Numer. Meth. Heat Fluid Flow*, **6**(1), 31-58, 1996.

[5] Raspo I, *Méthodes spectrales et de décomposition de domaine pour les écoulements complexes confinés en rotation*, Doctorate Thesis, Université de la Méditerranée, France, april 1996.

[6] Zanolli P., 'Domain decomposition algorithms for spectral methods', *Calcolo*, **24**, 202-240, 1987.

[7] Funaro D., Quarteroni A. and Zanolli P., 'An iterative procedure with interface relaxation for domain decomposition methods', *SIAM J. Numer. Anal.*, **25**(6), 1213-1236, 1988.

[8] Hugues S. and Randriamampianina A., 'An improved projection scheme applied to pseudospectral methods for the incompressible Navier-Stokes equations', *Int. J. Numer. Meth. Fluids* (to appear).

Smoothing techniques and approximation of invariant subspaces.

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1 Introduction

We are interested in computing the invariant subspace corresponding to a group of m_0 eigenvalues with smallest modulus of a nonsingular and nonsymmetric matrix operator D. As the typical operator, we consider some discrete models of elliptic differential operators obtained by finite element methods or with the help of difference schemes. Such finite dimensional models are described by large sparse $N \times N$ matrices. The methods used in the literature for solving this problem are often based on the shift-and-invert techniques combined with Krylov subspace methods [?]. This means that the solution of linear systems with the matrix D by Gaussian elimination or another direct method are required. As a consequence, the storage and the complexity requirement may be intolerably high.

We propose a method that avoids the computation of the action of D^{-1} on vectors. Along with the operator D, we use an additional operator K, which we can consider as a sparse matrix operator, i.e. the cost of the action of K on a vector x of dimension N is $O(N)$ arithmetical operations. The operator K must act as a *smoothing* operator whose ultimate aim is to remove the unrequired eigendirections. More precisely, the action of K on a given vector x will result in a vector y=Kx whose components in the smallest eigendirections dominate the other components.

The best results are obtained with a smoothing operator constructed iteratively as a one cycle of multi-grid iterations for approximating D^{-1}, not as the exact inverse of D.

The proposed method belongs to the family of projection methods [?]. i.e. methods based on the Petrov-Galerkin approximation. The construction is done in the spirit of the steepest descent method [?] and the Davidson method [?].

In the next section, we briefly describe our algorithm. We use the following notations : the symbol $v^{(*)}u$ denotes the inner product of N-dimensional vectors (or grid functions) u, v. The trace of a matrix A is denoted by $\mathrm{tr}(A)$. The notation $\mathrm{Span}\{X\}$ for a matrix X is used to denote the space spanned by the columns of X. A diagonal matrix of order n with diagonal elements $d_1, d_2, \ldots, d_n$ is denoted by $\mathrm{diag}\,(d_1, d_2, \ldots, d_n)$.

2 Algorithm

Let $\tilde{X}$ be an $N \times \tilde{m}$, $(\tilde{m} \geq m_0)$ matrix whose columns, or at least some of them, approximate an invariant subspace of D. The proposed iterative process begins by the construction of initial regular bases in the following way :

1. Form $Y = D\tilde{X}$ and $G = \tilde{Y}^{(*)}\tilde{Y}$.

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2. Perform an orthogonal diagonalization of the matrix $\tilde{G}$

$$\tilde{G} = \tilde{U}\ \mathrm{diag}\,(\tilde{g}_1, \tilde{g}_2, \ldots, \tilde{g}_{\tilde{m}})\ \tilde{U}^*, \quad \text{with} \quad \tilde{U}\tilde{U}^* = I_{\tilde{m}}, \quad \tilde{g}_1 \geq \tilde{g}_2 \geq \ldots \geq \tilde{g}_{\tilde{m}} \geq 0.$$

3. Calculate the practical dimension m that corresponds to the $\tilde{g}_k's$ which are larger that some prespecified tolerance.

4. From the first m columns of $\tilde{U} = \left(\tilde{u}^{(1)} \vdots \tilde{u}^{(2)} \vdots \ldots \vdots \tilde{u}^{(\tilde{m})}\right)$, construct the matrices

$$X = \tilde{X}\left(\tilde{u}^{(1)} \vdots \tilde{u}^{(2)} \vdots \ldots \vdots \tilde{u}^{(m)}\right) \mathrm{diag}\left(\frac{1}{\sqrt{\tilde{g}_1}}, \frac{1}{\sqrt{\tilde{g}_2}}, \ldots, \frac{1}{\sqrt{\tilde{g}_m}}\right) \quad \text{and } Y = DX.$$

Notice that the matrix Y satisfies the condition: $Y^{(*)}Y = I_m$.

After these steps, we calculate the $m \times m$ matrix

$$A = [X^{(*)}Y]^{-1}[X^{(*)}X]$$

which can be considered as an approximation of the operator D^{-1} on the subspace $\mathrm{Span}\{X\}$ in the sense that the matrix A^{-1} solves the matrix minimization problem

$$\min_B \mathrm{tr}\left((\mathrm{Y} - \mathrm{XB})^{(*)}(\mathrm{Y} - \mathrm{XB})\right).$$

Now, from the matrix residual $\Delta = Y - XA^{-1}$, we construct another rectangular matrix $\tilde{W}$ such that $\mathrm{Span}\{\tilde{W}\} \subset \mathrm{Span}\{\Delta\}$ and that the columns of $\tilde{W}$ correspond to the non converging vectors.

Finally, we refine the approximation of X by introducing the smoothing operator K. This is done by solving the matrix minimization problem

$$\min_C \mathrm{tr}\left((\mathrm{Y} - \mathrm{XA}^{-1} - \mathrm{KXCA}^{-1})^{(*)}(\mathrm{Y} - \mathrm{XA}^{-1} - \mathrm{KXCA}^{-1})\right).$$

It is important to notice that the use of $\tilde{W}$ only leads to a block Krylov type method whereas the use of $\tilde{W}$ and $\tilde{\tilde{W}}$ leads to a "preconditioned method" as in the Davidson method [?, ?].

We will examine in detail the mathematical properties of the above algorithm and show some numerical results when the operator K is constructed from multi-grid techniques. We also show some comparisons when K is constructed with the help of iterative methods such as GMRES.

References

[1] E.R. Davidson. The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17:87–94, 1975.

[2] S. K. Godunov, V. V. Ogneva and G. P. Prokopov. On the convergence of the modified steepest descent method in the calculation of eigenvalues. Amer. Math. Soc. Transl., 105:111–116, 1976.

[3] Y. Saad. Numerical methods for large eigenvalue problems. Algorithms and Architectures for Advanced Scientific Computing. Manchester University Press, Manchester, UK, 1992.

[4] M. Sadkane. Block Arnoldi and Davidson methods for unsymmetric large eigenvalue problems. Numer. Math., 64:195–211, 1993.

ICO98-10

Error estimates for Galerkin spectral discretizations of parabolic problems with non smooth data

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In this paper, we analyze the Legendre and Chebyshev Galerkin semi-discretizations to the homogeneous parabolic problem

$$\begin{aligned} u_t - (a(x)u_x)_x &= 0, \quad x \in \Lambda, t \geq 0, \\ u(-1,t) = u(1,t) &= 0, \quad t \geq 0, \\ u(x,0) &= u_0(x), \quad x \in \Lambda \end{aligned} \tag{1}$$

where $\Lambda = (-1,1)$, and a is a smooth function satisfying the classical assumption $0 < \underline{a} \leq a(x) \leq \overline{a}$ in $\overline{\Lambda}$, which ensures the parabolicity of the problem.

We denote by ω either the Legendre or the Chebyshev weight. We use the notations $L^2_\omega = \{v : \Lambda \mapsto \ | \int_\Lambda |v|^2 \omega dx < \infty\}$, $H^m_\omega = \{v \in L^2_\omega \mid d^j v/dx^j \in L^2_\omega, j = 1, \ldots, m\}$ and $H^1_{\omega,0} = \{v \in H^1_\omega, v(\pm 1) = 0\}$. We note by $\|\cdot\|_{m,\omega}$ the natural norm in H^m_ω.

The error estimates for spectral semi-discretizations of parabolic problems which can be found in litterature deal with the more general case of equations with a source term and need some amount of regularity of the initial condition. For instance, for the above problem, the assumption $u_0 \in H^m_\omega$ is made in order to get the estimate $\|u(t) - u^N(t)\|_{0,\omega} = O(N^{-m})$, where $u^N(t)$ stands for the solution of the semidiscrete Galerkin discretization. (See [3] and [2] for the constant coefficient case and [4] for the variable coefficient case). However, when the source term is null, we can expect, due to the regularization property of parabolic problems, that the same estimate will still hold under weaker assumptions on the regularity of the initial condition. Results of this kind have been obtained for finite element semidiscretization of parabolic problems: see [6], [7] and [8]. We do not know in litterature analogous results for spectral methods.

In this work, we take as discrete initial condition u_0^N the orthogonal projection (with respect to the inner product of L^2_ω) of u_0 over the space $\ ^N_0$ of the restrictions to Λ of the polynomials having degree at most N and vanishing at ± 1. We assume the function a to be smooth enough. We obtain the following results, where $e^N(t) = u(t) - u^N(t)$:

- For the Legendre discretization:

$$\|e^N(t)\|_{1,\omega} + N \|e^N(t)\|_{0,\omega} \leq C_m N^{-(m+1)} t^{-\frac{m+2}{2}} \|u_0\|_{0,\omega} \tag{2}$$

  for all $m \in \ , m \geq 1$, so that we have the spectral convergence (in spite of u_0 is just in L^2_ω).

- For the Chebyshev discretization:

$$\|e^N(t)\|_{0,\omega} \leq C N^{-\frac{5}{2}} t^{-\frac{5}{4}} \|u_0\|_{0,\omega} \tag{3}$$

$$\|e^N(t)\|_{1,\omega} \leq C N^{-\frac{5}{2}} t^{-\frac{7}{4}} \|u_0\|_{0,\omega} \tag{4}$$

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If $u_0 \in H^m_\omega$ and u_0 satisfies some additional boundary conditions when $m \geq 1$, then we have

$$\|e^N(t)\|_{1,\omega} + N \|e^N(t)\|_{0,\omega} \leq CN^{-(m+1)}t^{-1}\|u_0\|_{m,\omega} \tag{5}$$

There is a limit on the improvement of convergence which can be reached for initial data u_0 just in L^2_ω, even in the case $a(x) = 1$ over Λ. If we have for all $u_0 \in L^2_\omega$ a estimate of the form

$$\|e^N(t)\|_{0,\omega} \leq K(t, u_0)\, N^{-s} \tag{6}$$

then $s \leq \frac{7}{2}$.

The techniques used to obtain these results rely on semigroup theory, duality arguments and polynomial approximation results in weighted Sobolev spaces. (see [1] and [5].)

References

[1] C. Bernardi and Y. Maday, " Properties of some weighted Sobolev spaces and applications to spectral approximations ", *SIAM J. Numer. Anal.*, 26 (1989),pp. 769-829.

[2] C. Canuto, M.Y. Hussaini, A. Quarteroni and T.A. Zang, *Spectral methods in Fluid Dynamics*, Springer-Verlag, New York, 1988.

[3] C. Canuto and A. Quarteroni," Spectral and pseudo-spectral methods for parabolic problems with non periodic boundary conditions ", *Calcolo*, 18 (1981), pp 197-217.

[4] J. de Frutos Baraja y R. Muñoz Sola, " Chebyshev pseudospectral collocation for parabolic problems with nonconstant coefficients ", *Proceedings of the third international conference on spectral and high order methods*, Houston (Texas), (1996), 101-107.

[5] G. Fernández Manín y R. Muñoz Sola, " Polynomial approximation of some singular solutions in weighted Sobolev spaces ", *Proceedings of the third international conference on spectral and high order methods*, Houston (Texas), (1996), 93-99

[6] H. Fujita y T. Suzuki, *Evolution problems*, in *Handbook of numerical analysis, Vol. II*, eds. P. G. Ciarlet y J. L. Lions, North Holland, 1991.

[7] M. Luskin y R. Rannacher. " On the smoothing property of the Galerkin method for parabolic equations ", *SIAM J. Numer. Anal.*,19,(1982),93-113.

[8] V. Thomée, "Galekin finite element methods for parabolic problems ", *Lecture Notes on Mathematics*, 1054, (1984).

title: Compatibility Conditions for Time-Dependent Partial Differential Equations and the Rate of Convergence of Chebyshev and Fourier Spectral Methods

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Abstract

Compatibility conditions for partial differential equations (PDEs) are an infinite set of relations between the initial conditions, the PDE, and the boundary conditions which are necessary and sufficient for the solution to be infinitely differentiable everywhere on the computational domain including the boundaries.
Since the performance of Chebyshev spectral and spectral element methods is dramatically reduced when the solution is not infinitely differentiable, one would expect that the compatibility conditions would be a major theme in the spectral literature.
Instead, it has been completely ignored. Therefore, we pursue three goals in the paper. First, we present a proof of the compatibility conditions in a simplified form that does not require functional analysis. Second, we analyze the connection between the compatibility conditions and the rate of convergence of Chebyshev methods.
Lastly, we describe strategies for slightly adjusting initial conditions so that the compatibility conditions are satisfied.

ICO98-12

Time marching techniques for the nonlinear Galerkin method

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Abstract

In this article we study computational issues related to nonlinear Galerkin type splittings of dissipative partial differential equations in the case of a pseudospectral Fourier discretization.

The spacial semidiscretization of the equation is based on the decomposition of the unknown u into its large scale component y, represented by low Fourier modes, and small scale component z, represented by high Fourier modes. The use of projections on staggered coarse and fine grids allows the separation of modes in the collocation setting.

This separation of modes leads to the splitting of the original equation into two equations containing only low or high modes respectively Such a decomposition allows the use of distinct time integration techniques for each equation. In this paper we show how, by modifying the way the high modes are integrated, we can relax the stability constraint to that of the low modes allowing the choice of a much larger time step and resulting in a considerable reduction of the computational cost.

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The stability constraint of the high modes is determined by the size of the eigenvalues of the dissipative operator. The first technique consists in shifting the upper part of the spectrum through an exponential transformation in the z variable in conjunction with a high order Runge–Kutta scheme (ESRK). The choice of the parameter measuring the intensity of the shift is responsible for the improvement in the stability constraint and in the limit case will make the scheme for the high modes unconditionally stable. Unfortunately, this approach alters the steady state of the solution.

In the second part of this article we introduce two other modified Runge–Kutta schemes for the z variable based on an implicit polynomial correction. Both schemes preserve the steady state solution of the original problem.

However, the first scheme, NCIC, introduces an inconsistency in the approximation of the added time derivative term. The second scheme, CIC, uses a consistent implicit correction similar to the Du Fort–Frankel method, yielding a lower stability constraint while keeping the desired accuracy.

Numerical test are carried out for the periodic Burgers equation in one and two space dimensions, comparing the standard collocation scheme (SCM) with the collocation splittings coupled with the modified Runge–Kutta methods.

The tests show that, when the problem is strongly dissipative, the modified Runge–Kutta split methods produce an accurate solution using a time step four times larger than the one used by the standard approach, resulting in significant savings in the total computational cost. During the initial transient the CIC method performs slightly better than the NCIC and after the transient the solutions generated by the three methods are virtually indistinguishable.

We also experimented with low viscosity problems, where the advective part of the nonlinear term dominates the dynamic in the transient, creating a critical high gradient phase. Although in this case the high modes time step could not be improved significantly we observed that the separation of the modes allowed us to resolve and pass the critical phase using a smaller number of modes than the one required by the standard collocation approach. These preliminary results show the potential of this splitting techniques for applications to a broader class of problems.

Wavelets-based methods for numerical solution of nonlinear reaction-diffusion systems

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Abstract

Wavelet analysis [7, 10] was developed over last years and applications traditionally concern with signal and image processing. More recently, methods based on wavelets are applied to the numerical solution of partial differential equations (PDE's). This kind of methods has been studied both from the theoretical and the computational point of view, see for example, [6] for a review.
In particular, within the wavelet framework, we can realize an effective multiscale analysis of functions and operators [5]. A consequence consists in the possibility to build suitable fast and high order adaptive algorithms by using wavelet bases.
However some difficulties are not been (up to now) completely resolved: problems with complex geometry, efficient treatment of the nonlinear terms, and general boundary conditions. In order to overcome at least the last two difficulties, we consider here the collocation (pseudospectral) approach adopting interpolating multilevel bases [2]. Moreover, we consider the numerical simulation of reaction-diffusion type equations by using adaptive algorithms. In other words we approximate the solution of such a system in a sparse form. High resolution computations are performed only where the solution is not smooth and by looking at the size of the coefficients of our interpolating wavelet transform.Then adapted computational refinements are done near local singularities like, for example, sharp transition or shock wave. This means that we also assume that the solutions are smooth in a large part of the domain, while non smooth features appear locally.
For time dependent problems different numerical approaches can be used and coupled with wavelets in order to obtain a full discrete scheme. The three main approaches considered in this paper are the method of lines, the so-called Rothe method and the "semigroup approach".
The first one approach is based first on space then time discretization. After space approximation a system of ordinary differential equations (ODE'S), which is usually of stiff type, has to be solved numerically. Recently full discrete algorithms use linear-implicit time integration and some regridding space method.
In the Rothe method we take first time then space discretization: in this approach the PDE is understood as a differential equation in a suitable Hilbert space [8]. This permits one to use the well developed technology of the numerical methods for ODE's

and to treat the space discretization according to the accuracy bond required within each time layer.
Finally in the semigroup method !latexwe write the PDE as a nonlinear integral equation which then is approximate by using a suitable quadrature rule.
While for the method of lines [1, 9, 11], and for the semigroup approach [3, 4] some works have been done, Rothe-wavelet method is new [12].
These different approaches are considered with different numerical test together with some comparisons with respect to the "standard methods" (like finite differences or spectral methods). Moreover a preliminary stability analysis is given with some possible future development.

References

[1] S. Bertoluzza, *Adaptive wavelet collocation method for the solution of Burgers equation*, Transport Theory and Statisitcal Physics **25** (1996).

[2] S. Bertoluzza, G. Naldi, *A wavelet collocation method for the numerical solution of partial differential equations*, Applied and Computational Harmonic Analysis, Vol. **3** n.1, (1996).

[3] G. Beylkin, and J.M. Keiser,*On the adaptive numerical solution of nonlinear partial differential equations in wavelet bases*, preprint University of Colorado, Program in Applied Mathematics (1997).

[4] G. Chivassa, *Algorihtmes Adaptatifs en ondelettes pour la résolution d'equation aux dérivées partielles, Thesis Université de la Mediterranée Aix-Marseille II (1997).*

[5] W. Dahmen, *Wavelet and multiscale methods for operator equations*, Acta Numerica **7**, Cambridge University Press, pp. 55-228 (1997).

[6] W. Dahmen, A. Kurdila, P. Oswald, *Multiresolution analysis and wavelets for the numerical solution of partial differential equations.* Academic Press, (1997).

[7] I. Daubechies, *Ten lectures on wavelets.* SIAM Philadelphia, (1992).

[8] J. Lang, A. Walter, "A finite Element Method Adaptive in Space and Time for Nonlinear Reaction-Diffusion Systems". IMPACT Comput. Sci. Engrg. 4, 269-314 (1992).

[9] Y. Maday, V. Perrier, and J.C. Ravel, *Adaptivité dynamique sur bases d'ondelettes pour l'approximation d'équations aux dérivées partielles*, C.R. Acad. Sci. Paris, Ser. I **312**, (1991).

[10] Y. Meyer, *Hermann, Paris.* Ondelettes et operateurs, I: Ondelettes. (1990).

[11] G. Naldi, *Numerical Solution of Schrödinger equation: a Multilevel Approach*, preprint Pavia (1996).

[12] G. Naldi, *Apaptive Rothe wavelet methods for nonlinear reaction-diffusion system*, in preparation.

Wavelet-Galerkin Solution of Partial Differential Equations Applications to Data Assimilation

Andrew Tangborn* and **Sara Q. Zhang†**

We investigate the use of the wavelet-Galerkin method for solving partial differential equations with the goal of reducing the computational requirements of assimilating experimental data into CFD simulations. The Kalman filter is an optimal data assimilation scheme that determines the relative weighting of experimenatal and computational values that, when introduced into the simulation, produce the solution closest to the true state. Use of the Kalman filter requires the propagation of the state error covariance matrix, which is as yet impractical for multi-dimensional systems because of high computational costs. Recent efforts to approximate the propagation step have centered on representing the covariance matrix or the propagation matrix their eigendecomposition or SVD. We are developing similar techniques that make use of the wavelet expansion.

Wavelet representation of data is well know for its superior compression characteristics. This property can be exploited in the solution or multiplication of matrix systems by truncating the matrix represented in wavelet space. For example, if we apply the wavelet operator W to a covariance matrix P,

$$\hat{P} = W^T P W$$

to obtain the projection of the covariance matrix onto a wavelet basis, we get a sparse matrix with just a few non-negligible terms on the main diagonal. Multiplication of this matrix by the propagation matrices can be severely truncated without significant loss of information.

Representation of the error covariance and error propagation matrices in wavelet space requires that the PDE also be solved using wavelet representation. We demonstrate these techniques on the convection-diffusion equation using a compactly supported wavelet basis. A Gaussian error covariance matrix is assumed and propagated using wavelet representation. A range of degrees of truncation of the system are carried out and comparisons in accuracy with the full system are made.

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A General Adaptive Solver for Hyperbolic PDEs Based on Filter Bank Subdivisions

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There are results from wavelet theory that are promising if we wish to construct fast solvers for hyperbolic PDEs. Especially, the idea that the regularity of a function (in terms of its Hölder exponent) is completely characterized by the magnitude of the coefficients of its wavelet expansion [2] seems useful.

As the solutions of hyperbolic equations often are smooth except for some small regions with sharp gradients (or even discontinuities in the non-viscous case), and the wavelet coefficients only depend on the *local* regularity of a function, we can expect such a solution to have a sparse representation in a wavelet basis, at least if we decide some threshold-value below which we set coefficients to zero (so called ϵ-thresholding).

However, the straightforward implementation of such a sparse solver, using a Galerkin method tends to be inefficient as shown, e.g., in [1]. This is true especially for non-linear equations, as multiplication is non-trivial in the wavelet domain. The constants in the asymptotic complexity estimates are simply too large for numerical efficiency.

These difficulties inspired the development of the *filter bank method.* The idea is to "split" the solver into two parts: *the operator part,* for which finite difference approximations are used, and *the representation part* where the filter bank transform (which is the discrete version of the wavelet transform) is used.

Ideally, the operator part of the solver would be constructed taking into consideration the questions of stability and order of approximation and then the representation part, which is very much the same regardless of the problem, is "hooked onto the solver" to give adaptivity.

This approach of "splitting" the solver, switching from the wavelet to the filter bank transform for the representation part and using finite difference methods for the operator part has a number of advantages as shown in [3]. The most crucial are

- With the right filter banks, multiplication of functions becomes trivial.
- Short filters that may not correspond to any wavelets (at least not in the classical sense) can be used, leading to faster solvers.
- The automatic scale decomposition and detection of sharp gradients makes it simple to use different solvers in different parts of the domain (e.g. adding viscosity terms only in a neighborhood of boundary layers).
- A minimum amount of extra work is needed at boundaries due to short filters.
- The idea is easily extended to non-Cartesian domains as shown in [4].

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A discrete version of the implication: local Hölder regularity $\Rightarrow$ local sparse representation was also derived in [3] giving a theoretical justification to this discrete approach.

We use the proposed method to solve some non-trivial equations in one and two dimensions; namely the Euler and the Navier-Stokes equations. We are especially interested in answering the following questions:

- How well separated are the operator and the representation problems? Is it "easy" to hook the filter bank part onto an arbitrary problem? As the program is written in C++, this would capture the important object-oriented properties of encapsulation and code reuse.
- How robust is the method? Can we solve a large set of problems without having to "fine-tune" parameters?
- What is the break-even problem size between the adaptive method and the non-adaptive method (i.e. the pure finite difference solver)? How far have we brought down the complexity constants by using the discrete method?

The presented examples will show the strengths and weaknesses of the filter bank method.

References

[1] M. Holmström and J. Waldén. Adaptive wavelet methods for hyperbolic PDEs. Technical Report 171, Dept. of Scientific Computing, Uppsala University, Box 120, Uppsala, Sweden, 1995.

[2] Y. Meyer. *Wavelets and operators.* Cambridge University Press, 1992.

[3] J. Waldén. Filter bank methods for hyperbolic PDEs. Technical Report 185, Dept. of Scientific Computing, Uppsala University, Box 120, Uppsala, Sweden, 1996.

[4] J. Waldén. Filter bank subdivisions of bounded domains. Technical Report 196, Dept. of Scientific Computing, Uppsala University, Box 120, Uppsala, Sweden, 1997.

Presenter:
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Title:
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Spectral methods for boundary-value problems based on non-classical orthogonal polynomials.

Abstract:
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Spectral methods for solving boundary-value problems numerically have traditionally been based on classical orthogonal polynomials such as Chebyshev, Laguerre, and Hermite. In this talk we investigate the potential advantages of spectral methods based on non-classical orthogonal polynomials.

Numerical examples include:

(1) The solution of a Sturm-Liouville problem on the real line by a spectral method based on orthogonal polynomials generated by the logistic density weight function.

(2) The solution of a boundary-value problem with a steep boundary layer by a method based on orthogonal polynomials generated by a rational weight function. The method may be viewed as a spectral method based on a rational interpolant with pre-assigned poles. The poles are chosen to mimic the almost singular behavior of the solution.
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Discrete-Time Orthogonal Spline Collocation Methods for Vibration Problems

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Abstract

We consider discrete–time orthogonal spline collocation (OSC), that is, spline collocation at Gauss points, methods for the approximate solution of the equation

$$\frac{\partial^2 u}{\partial t^2} + 2\nu\frac{\partial u}{\partial t} + \Delta(q(x,y)\Delta u) = f(x,y,t), \quad (x,y,t) \in \Omega_T \equiv \Omega \times (0,T],$$

where ν is a nonnegative constant related to viscous damping coefficient ($\nu = 0$ if external viscous damping is ignored), Δ is the Laplacian, $q(x,y)$ is a variable density function such that

$$0 < q_{\min} \le q(x,y) \le q_{\max} < \infty, \quad (x,y) \in \Omega,$$

and $\Omega = (0,1) \times (0,1)$ with boundary $\partial\Omega$. This equation commonly arises in plate vibration and seismological problems. The initial conditions are

$$u(x,y,0) = g_0(x,y), \quad \frac{\partial u}{\partial t}(x,y,0) = g_1(x,y), \quad (x,y) \in \overline{\Omega},$$

while the boundary conditions (BCs) are of one of the following three types:
BC1: "clamped" BCs:

$$u(x,y,t) = 0, \quad \frac{\partial u}{\partial n}(x,y,t) = 0, \quad (x,y,t) \in \partial\Omega \times (0,T],$$

where $\partial/\partial n$ is the outward normal derivative:
BC2: "hinged" BCs:

$$u(x,y,t) = 0, \quad \Delta u(x,y,t) = 0, \quad (x,y,t) \in \partial\Omega \times (0,T];$$

BC3: BCs in which the vertical sides are hinged and the horizontal sides are clamped:

$$\begin{aligned} u(x,y,t) &= 0. \quad (x,y,t) \in \partial\Omega \times (0,T], \\ \Delta u(x,y,t) &= 0. \quad (x,y,t) \in \partial\Omega_1 \times (0,T], \\ \frac{\partial u}{\partial n}(x,y,t) &= 0. \quad (x,y,t) \in \partial\Omega_2 \times (0,T]; \end{aligned}$$

where

$$\partial\Omega_1 = \{(\alpha,y) : \alpha = 0,1,\ 0 \le y \le 1\}, \quad \partial\Omega_2 = \{(x,\alpha) : 0 \le x \le 1,\ \alpha = 0,1\}.$$

We reformulate each problem by introducing the functions

$$u_1 = e^{\nu t}\frac{\partial u}{\partial t}. \qquad u_2 = qe^{\nu t}\Delta u.$$

For example, setting

$$U = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad F = \begin{bmatrix} e^{\nu t} f \\ 0 \end{bmatrix}, \quad G = \begin{bmatrix} g_1 \\ q\Delta g_0 \end{bmatrix},$$

in the problem with BC1, we obtain the Schrödinger system

$$\begin{cases} \dfrac{\partial U}{\partial t} - S_q \Delta U + \nu R U = F, & (x,y,t) \in \Omega_T, \\ U(x,y,0) = G(x,y), & (x,y) \in \Omega, \\ u_1(x,y,t) = 0, \ \dfrac{\partial u_1}{\partial n}(x,y,t) = 0, & (x,y,t) \in \partial\Omega \times (0,T], \end{cases}$$

where

$$S_q = \begin{bmatrix} 0 & -1 \\ q & 0 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Note that it is necessary to carry out an additional calculation to obtain an approximation to u from that to u_1.

To determine an approximation to U, we use OSC with C^1 piecewise polynomials of arbitrary degree $r \geq 3$ in each space variable for the spatial discretization. The resulting systems of ordinary differential equations in the time variable are then discretized using standard Crank–Nicolson or alternating direction implicit (ADI) techniques involving only two time levels (cf. [1]). Specifically, we formulate and analyze Crank–Nicolson OSC schemes for all three choices of BCs, and also formulate ADI OSC methods for BC2 and BC3 and analyze these methods for the special case in which q is a constant and $\nu = 0$. Based on our experience with OSC methods for the biharmonic Dirichlet problem [2], we believe that it is not possible to formulate a standard ADI method for BC1. For this problem, we employ the capacitance matrix method to solve the Crank–Nicolson scheme efficiently for the the special case of constant q and C^1 piecewise bicubic polynomials on a uniform partition of Ω. We examine the existence, uniqueness and stability of each scheme and show that, for each, the H^m-norm, $m = 1, 2$, of the error at each time step is of optimal order $r + 1 - m$ in space and second order in time. Implementational issues are discussed and numerical results are presented which confirm the theoretical analyses.

[1] B. Li, G. Fairweather and B. Bialecki, *Discrete-time orthogonal spline collocation methods for Schroödinger equations in two space variables*, SIAM J. Numer. Math., 35 (1998), to appear.

[2] Z.-M. Lou, B. Bialecki and G. Fairweather, *Discrete-time orthogonal spline collocation methods for biharmonic problems*, Numer. Math., to appear.

A 3-D Spectral Methods Approach to Simulation of Particle Motion in Fluids

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The study of the interaction of particle motion with fluid motion in laminar and turbulent flows is of special interest not only for the understanding of the underlying physics but also for practical applications. Understanding of the interaction and the motion of particles is especially important for mixing processes, sedimentation and applications that involve boiling or other two-phase flows. In this work, we are interested in simulating the motion of particles in a fluid between two parallel plates in order to determine the interactions between the particles and the fluid in 3-D. We consider two-dimensional and three-dimensional, horizontal or vertical fluid layers heated uniformly from below or unheated. Particles are introduced at different locations and we observe their interactions with the fluid motion.

Numerical simulations of two-phase flows are generally classified as Eulerian, where the transport equations are solved separately for two continuous phases; or Lagrangian, where only the liquid phase is solved as a continuum and the gas phase is represented by a large number of particles whose motion is determined by calculating the net forces on each individually. There have been extensive work done on two-phase flow using the Lagrangian approach, showing, for example, that turbulent flow fields tend to slow the rise of bubbles. Heavy particles (or aerosols) tend to be unaffected by the flow field if they are large. They act as passive scalars if they are very small. In a mid range

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of sizes, heavy particles are scattered most widely by the large scale vortices in the flow.

Our approach to the stated problem involves simulation of both the fluid motion and the motion of the particles by using a 3-D spectral technique. Non-dimensional forms of the full Navier-Stokes and the energy equations (N-S) are solved with a spectral algorithm incorporating a Fourier expansion in the periodic streamwise direction and a Fourier-Chebychev expansion in the vertical direction. The motion of the particles are modeled with Small Spherical Particle Equation of Motion (EOM) in the form formulated by Maxey and Riley [1].

The solutions of these two sets of equations are two-way coupled by incorporating in EOM the fluid velocities and their derivatives from the solution of N-S. In turn, the surface forces of EOM are included as localized body forces in N-S. The forces on individual particles are calculated via an interpolation of the Chebychev and Fourier expansions, while a weighting scheme is used to impose forces from particles in N-S. We assume that the particles, which behave as rigid spheres, are very small so that the Reynolds number based on particle diameters is small. We further assume that there are no interactions between particles, except if two come into contact, they combine, with the volumes added together. Also, interactions between the particles and the channel walls are not considered.

Simulations have been carried out in 3-D with a variety of particle sizes and density ratios. Two very different cases has been considered to apply our approach: the first one involves particles in a horizontal flow in a heated channel; and the other simulates the wake-induced motion of bubbles in a vertical channel. Both cases also include the simplified version of coalescence of bubbles or joining of touching particles.

[1] Maxey, M.R., J.J. Riley, 1983, "Equation of motion for a small rigid sphere in a nonuniform flow", *Physics of Fluids, A.*, Vol. 4, pp. 883–889.

Compatible Approximation Spaces for the Velocity-Pressure-Stress Formulation for Creeping Flows

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Abstract

The most popular and almost universally used formulation of the governing equations of viscoelastic flow is in terms of velocity, pressure and extra-stress. Unlike the situation in Newtonian fluid mechanics the extra-stress tensor cannot be eliminated from the equation of motion to obtain a formulation solely in terms of velocity and pressure. This is due to the nonlinear stress-strain relationship. The motivation for this work is governed by a desire to generate well-posed approximations to viscoelastic flow problems using spectral methods. One of the most fundamental questions concerning the formulation of the associated discrete problem is what is the most appropriate choice of approximation spaces.

It is well-known for the classical velocity-pressure formulation of the Stokes problem that the corresponding discrete approximation spaces must satisfy a compatibility condition to ensure the problem is well-posed. This is the so-called Babuška-Brezzi condition. Maday and Patera [2] have shown that a suitable choice for the pressure approximation space is $P_{N-2}(\Omega)$ if the velocity approximation space is $P_N(\Omega)$. Here $P_K(\Omega)$ is the space of polynomials of degree K or less in each coordinate direction in some bounded domain Ω. This choice leads to an optimal error estimate for the velocity in model geometries.

The discretization of viscoelastic flow problems by spectral methods requires the choice of an additional approximation space - for the extra-stress. A number of researchers have investigated computationally the most appropriate choice for this space for smooth and nonsmooth problems. Suppose that the extra-stress and velocity fields are approximated by polynomials of degree N_T and N_v, respectively. Talwar and Khomami [4] have shown for the flow past a square array of cylinders that $N_T \geq N_v - 1$ is required to avoid spurious oscillations in the velocity field. In fact they suggest $N_T = N_v$ and this has obvious advantages from the point of view of implementation since no interpolation is required between the velocity and extra-stress grids. For the flow through an undulating tube Van Kemenade and Deville [5] have shown that one should choose N_T such that $N_v \leq N_T \leq N_v + 2$. They also show that convergent approximations for a slightly larger range of Deborah numbers are achieved when $N_T = N_v + 2$. However, this small gain in robustness hardly seems worth the extra computational effort. Although some of these

results are contradictory it is clear that an under-discretization of the extra-stress can result in spurious oscillations in the velocity field.

In this paper we show theoretically that for a single spectral element a necessary condition for the discrete Stokes problem to be well-posed is $N_T \geq N_v$. Furthermore, if $N_T = N_v$ then optimal error estimates can be derived for the velocity and extra-stress. The convergence analysis requires the satisfaction of a second compatibility condition, this time between the discrete velocity and extra-stress spaces. Marchal and Crochet [3] have shown that the velocity-pressure and velocity-pressure-stress formulations of the Stokes problem gave different results unless the stress approximation is chosen correctly in the Galerkin formulation. In particular, for the stick-slip problem the latter formulation gave rise to spurious oscillations in both the velocity and stress fields. Fortin and Pierre [1] also require the satisfaction of this second compatibility condition in their analysis of the so-called 4×4 element of Marchal and Crochet [3] which is constructed by subdividing the biquadratic extra-stress element into 4×4 bilinear stress elements.

The choice of the discrete stress space in the spectral element context is motivated in two ways. First of all by consideration of the properties of the solution of the variational statement of the velocity-pressure-stress formulation of the Stokes problem. Since the components of the extra-stress tensor are functions in $L^2(\Omega)$ it seems reasonable to allow the stress to be continuous between elements. Secondly, by looking at an appropriate way of matching the discrete solution between elements to ensure that the global compatibility condition is not violated. Suppose we employ an approximation for the extra-stress which is continuous between elements. If we pursue this approach we obtain the following contradiction. Suppose that $\tau_N \in \mathcal{T}_N$ and $\vec{v}_N \in \mathcal{V}_N$, then since

$$\tau = 2\eta \boldsymbol{d},$$

we have that $\boldsymbol{d} \notin \mathcal{T}_N$, in general. Therefore a sufficient condition for compatibility between the velocity and stress approximation spaces is

$$\vec{v}_N \in \mathcal{V}_N \Rightarrow \left(\vec{\nabla}_N \vec{v}_N + \left(\vec{\nabla}_N \vec{v}_N \right)^T \right) \in \mathcal{T}_N,$$

where $\vec{\nabla}_N$ is the discrete gradient operator. This condition is satisfied if the stress tensor is allowed to be discontinuous. Numerical results are presented for smooth and nonsmooth problems showing the consequences of satisfying or violating this condition.

References

[1] M. Fortin and R. Pierre. On the convergence of the mixed method of Crochet and Marchal for viscoelastic flows. *Comput. Meth. Appl. Mech. Engrg*, 73:341–350, 1989.

[2] Y. Maday and A. T. Patera. Spectral element methods for the incompressible Navier-Stokes equations. In A. K. Noor and J. T. Oden, editors, *State of the Art Surveys in Computational Mechanics*, pages 71–143, New York, 1989. ASME.

[3] J. M. Marchal and M. J. Crochet. A new mixed finite element method for calculating viscoelastic flow. *J. Non-Newtonian Fluid Mech.*, 26:77–114, 1987.

[4] K. K. Talwar and B. Khomami. Application of higher order finite element methods to viscoelastic flow problems in porous media. *J. Rheol.*, 36:1377–1416, 1992.

[5] V. Van Kemenade and M. O. Deville. Application of spectral elements to viscoelastic creeping flows. *J. Non-Newtonian Fluid Mech.*, 51:277–308, 1994.

where B is the Biot number.

$\underline{x=-1}$

$$T=1,\ \psi=0,\ \partial_x\psi=0,\ \partial^2_{x^2}\psi=0, \tag{8}$$

$\underline{x=1}$

$$T=\frac{T_c-T_a}{T_u},\ \psi=0,\ \partial_z v=0,\ \partial^2_{x^2}\psi=0, \tag{9}$$

We have solved numerically these equations with a Chebyshev-Collocation method. The solution is a stationary state that consists of a transverse roll or several ones. We have studied the linear stability of this solution perturbing it and solving the corresponding eigenvalue problem. The result of this analysis is that longitudinal rolls appear after a stationary bifurcation of the transverse ones. The threshold in the horizontal temperature gradient for such bifurcation depends on the temperature in the wall opposite to the heated one, on the depth of the layer, on its width and on the coefficient of heat exchange with the atmosphere. These results coincide with the observed in recent experiments.

The convergence results for the method are summarized in the following tables:

Table I

Some meaningful states. T_c is the temperature of the cold wall and T_a the ambient temperature.

State	$T_c - T_a$(°C)	l(cm)	d(mm)
A	-1	6	2.5
B	1	6	2.5
C	-1	6	1.5
D	-1	7	1.5

Table II

Critical temperature gradient for the different states described in the table I at consecutive orders in the development in Chebyshev polynomials.

State	6×20	7×21	8×22	9×23	Relative error
A	5.34	5.30	5.29	5.28	0.2 %
B	2.63	2.58	2.55	2.59	1.5 %
C	21.48	21.15	21.06	20.96	0.5 %
D	20.65	20.59	20.54	20.49	0.2 %

References

[1] A.M. Mancho, H. Herrero and J. Burguete. Phys. Rev. E **56**, 2916 (1997).

[2] H. Herrero and A.M. Mancho. Submitted to Phys. Rev. E.

Instabilities in a lateraly heated liquid layer

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Abstract

We study the stability of convective motions generated by heating laterally a layer of a liquid finite in the direction of the gradient (l) and in the vertical one (d), and infinite in the other dimension, with the upper surface opened to the atmosphere and taking into account effects of buoyancy and thermocapillarity. The equations for the balances of moment and energy in the stationary state are:

$$a\partial^2_{zx}\psi\partial_x T - \partial^2_{x^2}\psi\partial_z T = \Delta T, \quad (1)$$

$$\Delta\Delta_2\partial^2_{x^2}\psi - \frac{1}{2}R\partial^2_{x^2}T = 0, \quad (2)$$

where $u = \nabla\times\nabla\times\psi e_z$ is the velocity, T is the temperature, $\Delta = a\partial^2_{x^2} + \partial^2_{z^2}$, $\Delta_2 = \partial^2_{x^2} + \partial^2_{z^2}$, R is the Rayleigh number and $a = d^2/l^2$.

The boundary conditions are

$\underline{z = -1}$

$$\psi = 0, \ \partial_z\psi = 0, \quad (3)$$

$$T = 1 - \frac{c}{2}(x+1). \quad (4)$$

where c depends on the different temperatures involved in the problem.

$\underline{z = 1}$

$$\psi = 0, \quad (5)$$

$$\partial^2_z\partial_x\psi + M\partial_x T = 0, \quad (6)$$

eq. (6) is the viscosity condition in the free surface, where M is the Marangoni number that describes the effects of thermocapilarity.

$$BT = -2\partial_z T, \quad (7)$$

Flow Past a Cylinder using a Semi-Lagrangian Spectral Element Method

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Abstract

The flow past a cylinder symmetrically positioned between two parallel plates is one of the current benchmark problems in viscoelastic flow. This problem is used to test the accuracy and robustness of numerical methods and to compare results of numerical simulations with experimental observations in order to assess the reliability of constitutive models. The dependence of the drag on the cylinder as a function of Reynolds number (Re) and Weissenberg number (We) is of importance and is used to compare the accuracy of competing numerical methods.

Although there are no geometrical singularities in the problem there are numerical difficulties associated with the resolution of boundary layers on the cylinder. These become increasingly thin with increasing elasticity. Our choice of the spectral element method [4, 3] to solve this problem is motivated by the need to resolve these boundary layers since we can arrange the spectral elements so that there is a high concentration of grid points near the surface of the cylinder.

The computational domain is divided into a number of spectral elements each of which is mapped on to a parent element using a transfinite mapping technique [2]. A time splitting scheme is used in which the convection terms in in the momentum and constitutive equations are treated using a semi-Lagrangian approach. The remaining terms in the momentum equation are treated implicitly in a a generalized Stokes step. The semi-Lagrangian approach is sometimes known as the operator-integration-factor splitting method [5] or the method of characteristics [1]. This is a stable and efficient way of treating the convection term which is so often the bane of numerical methods for convection-dominated problems. A second order in time variant of the mehod of characteristics is used here in which the characteristic equations are solved using the fourth-order explicit Runge-Kutta method. The variational formulation of the generalized Stokes problem follows standard spectral element practice [3, 6] so that at the end of each time step the velocity field is divergence-free in a weak sense.

Numerical results demonstrate the convergence of the pseudospectral approximations with respect to the order of polynomial approximation, positions of element interfaces and the length of the downstream section. Comparisons are made with other methods by comparing the calculation of the drag.

The drag decreases sharply from its value for $Re = 0$ as soon as inertia is introduced. It continues to decrease as Re increases further.

References

[1] K. Boukir, Y. Maday, B. Metivet and E. Razafindrakoto. A high order characteristics/finite element method for the incompressible Navier-Stokes equations, Int. J. Numer. Meth. Fluids **25** (1997), 1421-1454.

[2] W. J. Gordon and C. A. Hall. Construction of curvilinear coordinate systems and application to mesh generation, Int. J. Numer. Meth. Eng. 7 (1973), 461-477.

[3] Y.Maday, D.Meiron, A.T.Patera and E.M.Rønquist Analysis of iterative methods for the steady and unsteady Stokes problem: application to spectral element discretizations, SIAM J. Sci. Comput. **14 (1993), 310-337.**

[4] Y.Maday and A.T.Patera. Spectral element methods for the incompressible Navier-Stokes equations. In: State of the Art Surveys in Computational Mechanics (A.K.Noor and J.T.Oden, Eds.), 1989, 71-143.

[5] Y.Maday, A.T.Patera and E.M.Rønquist. An Operator-Integration-factor splitting method for time-dependent problems. Application to incompressible fluid flow, J. Sci. Comput. **5** (1990), 263-292.

[6] Y.Maday, A.T.Patera and E.M.Rønquist. The $P_N - P_{N-2}$ method for the approximation of the Stokes problem, submitted to Numer. Math. (1993).

An accurate and efficient spectral method for studies of the dynamical properties of forced, circular shear layers

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Abstract

In the study of the nonlinear dynamics of coherent structures, which are important in many flow systems of practical relevance, forced circular shear flows offer many desirable features. The inherent quantization of circular geometries due to the periodic boundary conditions makes it possible to design experiments in which the spatial and temporal complexity of the coherent structures can be accurately controlled. A large number of experiments on circular shear layers have been performed in a variety of physical systems, including rotating gases and fluids, and magnetized plasmas. A number of theoretical and numerical investigations of these systems have also previously been performed. However, the quantitative agreement between the results from these theoretical and numerical studies and the experimental results has been rather poor, mainly due the low order of the numerical methods employed.

We have developed an accurate and efficient Fourier-Chebyshev method for numerical investigations [1,2] of the dynamical properties of forced, circular shear layers. This method is used both in full temporal simulations of the flow system and in a theoretical/numerical asymptotic expansion of the dynamical equations in the near-linear regime. The dynamical system is modeled by the incompressible Navier–Stokes equations in the vorticity–stream function (ω–ψ) formulation. The external forcing is expressed by a term proportional to $\omega(r,\theta,t) - \omega^*(r)$, where $\omega^*(r)$ is a fixed forcing function. Compared to the primitive variable approach, the ω–ψ formulation reduces the number of dynamical equations from two to one, it eliminates the pressure from the calculations and the incompressibility condition, $\nabla \cdot \mathbf{u} = 0$, is satisfied by construction. However, no-slip boundary conditions cause the Poisson equation relating ψ to ω to be overdetermined. We have previously developed an integral solvability constraint method [3] to resolve the apparent overdeterminancy. In this method, the coefficients belonging to the solvability constraints are independent of viscosity and mode number truncation, and they are calculated in a pre-processing stage. This way, imposing the solvability constraints during the dynamical calculations add virtually no computational overhead. In order to determine the effects of the bounding walls, the model equations are also solved for free-slip boundary conditions.

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For the time integration of the dynamical equations, we have used a 3rd order 'Stiffly-Stable' scheme [4], which is a mixed explicit/implicit time-integration method. Thus, for each time-step two elliptic equations, the Poisson equation relating ψ to ω and the Helmholtz equation originating from treating the viscous terms implicitly, must be solved. For the solution of these linear equations, the fast and accurate invertible integral operator method [5] is used. In the explicit calculation of the nonlinear convection term, the products are calculated in point space and the result fully de-aliased using the standard 2/3 truncation scheme. The accuracy of the full numerical simulations is diagnosed by comparing the instantaneous temporal derivatives of the global quantities: energy, enstrophy and angular momentum, obtained by time-stepping the simulation, with the analytical expressions for these quantities, and very high accuracies are obtained.

The results from the full simulations at low Reynolds numbers are compared with results from the linear stability analysis and are also used to give predictions for the coefficients of the Landau equation describing the saturation behavior near the critical Reynolds number. As part of the linear stability characterization, the pseudo-spectrum for the associated Orr–Sommerfeld operator for plane, circular Couette flow is calculated and is found to be insensitive to perturbations. Numerical results at higher Reynolds numbers give the first non-experimental account of the effects of spin-up and spin-down, including the experimentally observed hysteresis. The properties of two-dimensional shears at high Reynolds numbers, at which temporal states are formed, have also been addressed.

The numerical results are validated both qualitatively and quantitatively through detailed comparisons with experiments carried out in rotating flows with planar [6] and parabolic [7] geometries. In the later case, the dynamical equations are extended to include the effect of a radially varying Coriolis force (the 'beta' effect).

References

[1] K. BERGERON, E.A. COUTSIAS, J.P. LYNOV AND A.H. NIELSEN, *Self-organization in circular shear layers.* Physica Scripta **T67**, 33-37 (1996).

[2] K. BERGERON, E.A. COUTSIAS, J.P. LYNOV AND A.H. NIELSEN, *Dynamical properties of forced shear layers in an annular geometry.* Submitted for publication.

[3] E.A. COUTSIAS AND J.P. LYNOV, *Fundamental interactions of vortical structures with boundary layers in two-dimensional flows.* Physica D **51**, 482-497 (1991).

[4] G.E. KARNIADAKIS, M. ISRAELI AND S.A. ORSZAG, *High-order splitting methods for the incompressible Navier–Stokes equations.* J. Comput. Phys. **97**, 414-443 (1991).

[5] E.A. COUTSIAS, T. HAGSTROM AND D. TORRES, *An efficient spectral method for ordinary differential equations with rational function coefficients.* Math. Comp. **65**, 611-635 (1995).

[6] J.M. CHOMAS, M. RABAUD, C. BASDEVANT AND Y. COUDER, *Experimental and numerical investigation of a forced circular shear layer.* J. Fluid Mech. **187**, 115-140 (1988).

[7] J.A. VAN DE KONIJNENBERG, A.H. NIELSEN, J. JUUL RASMUSSEN AND B. STENUM, *Shear flow instability in a rotating fluid.* Submitted for publication.

Fast 3-D Spectral Elliptic Solver of Arbitrary Order Accuracy Using Fourier Series

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Key words. 3-D solver for the Poisson and Helmholtz equations, Dirichlet problem, mixed problem, Fourier method.

AMS subject classifications. 65N35, 65T20

Fast and accurate solution of elliptic equations is an important step for problems arising in computational physics or fluid dynamics.

We present a direct solver for the Poisson, Laplace and Helmholtz equations in a 3-D cube. The method is based on the application of the discrete Fourier transform accompanied by a subtraction technique which allows to reduce the errors associated with the Gibbs phenomenon and achieve any prescribed rate of convergence. The algorithm requires $O(N^3 \log N)$ operations, where N is the number of grid points in each direction.

We consider the Poisson equation

$$\Delta u = f \tag{1}$$

with Dirichlet boundary conditions.

First, a particular solution of (1) is obtained, then an auxiliary problem for the Laplace equation is solved. The boundary conditions for the auxiliary problem are obtained as the difference between the original boundary conditions and those obtained from the particular solution. If the particular solution corresponds to zero boundary values, then we solve the Laplace equation with the original boundary conditions.

Thus, the algorithm consists of two steps:

Step 1. Solving a Poisson Eq. (1) with some boundary conditions;

Step 2. Solving a Laplace equation with with specified boundary conditions.

The Fourier method has the following advantages when solving the Poisson (Helmholtz) equation: first, differential operators are represented in the Fourier basis by diagonal matrices, second, for infinitely differentiable and periodic functions the approximation by Fourier series converges more rapidly than any finite power of $1/N$, where N is the number of Fourier harmonics.

If the function f or/and boundary conditions are non-periodic, then a special technique is necessary to reduce the Gibbs phenomenon; otherwise the Fourier series converges as $1/N$, with N being a number of points in each direction. Below we describe two steps of the algorithm and characterize the methods used to avoid the Gibbs phenomenon.

1. The function f in the right hand side of Eq. (1) is extended to a larger domain and it is replaced by a new function which coincides with f in the original domain and it is periodic together with a certain number of its derivatives in the larger domain. This procedure is due to Local Fourier Basis method which is described in [2].

2. The auxiliary boundary value problem for the Laplace equation is solved to satisfy the original boundary conditions. We reduce the effect of the Gibbs phenomenon by employing the subtraction technique similar to [1] where it was applied to 2-D case. The boundary conditions are represented as a sum of periodic functions and functions being a restriction of the known harmonic functions to the boundaries.

Similar procedure is applied to the edges. Finally, the solution is derived by the application of the Discrete Sine Transform to each of the six faces, where the boundary conditions are eventually periodic.

A similar algorithm for the 2-D case was developed and implemented in [1]. However in 3-D the geometry is more complicated: in 2-D the only subtraction step was concerned with the corners, while in 3-D we have to treat both corners and edges.

Numerical results demonstrate fast convergence and high accuracy of the method. For example, if after the subtraction procedure the boundary conditions are periodic together with the three first derivatives, then for the right

hand side

$$f(x,y,z) = exp\left\{-3((x-0.5)^2 + (y-0.5)^2 + (z-0.5)^2)\right\}$$

the accuracy of 10^{-8} is achieved only for 16 grid points in each direction (8 points in each direction are used for the extension), while for the right hand side $f(x,y,z) = \cos x \cos y \cos z$ this number of points gives the accuracy of 10^{-9}. The complete results are presented in [3].

We show that our approach allows accurate treatment of singular cases which arise when the boundary function is discontinuous or incompatible with the differential equation.

The fast solver is also generalized to the Helmholtz equation

$$\Delta u + \lambda u = f \tag{2}$$

with λ being positive or negative.

It is also demonstrated how the method changes when the Neumann/mixed problem is solved instead of the Dirichlet problem for elliptic equations.

References

1. A. Averbuch, M. Israeli, L. Vozovoi, A Fast Poisson Solver of Arbitrary Order Accuracy in Rectangular Regions, to appear in *SIAM J. of Scientific Computing.*
2. L. Vozovoi, M. Israeli and A. Averbuch, Spectral multi-domain technique with Local Fourier basis II: decomposition into cells, *J. Sci. Comput.* **9**, 311-326 (1994).
3. E. Braverman, M. Israeli, A. Averbuch and L. Vozovoi, A Fast 3-D Poisson Solver of Arbitrary Order Accuracy, submitted J. of Computational Physics.

On compact high order finite difference schemes

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The general approach for construction of the fourth order compact approximations of partial differential equations (PDE's) is applied for two- and three-dimensional (2D& 3D) Dirichlet boundary value problems (BVP). The uniform rectangular and parallelepipedoidal grids are used in 2D and 3D problems respectively. The solutions of BVP are supposed to be smooth enough. The stationary and non-stationary problems are investigated for the second order PDE's of elliptic, parabolic and hyperbolic types with constant or variable coefficients, including anisotropy.

For 2D diffusion-convection equation

$$Lu = (L_x + L_y)u \equiv -\frac{\partial}{\partial x}p\frac{\partial u}{\partial x} + a\frac{\partial u}{\partial x} - \frac{\partial}{\partial y}q\frac{\partial u}{\partial y} + b\frac{\partial u}{\partial y} = f,$$

we define the set of nine-point schemes

$$L^h u \equiv L^h_{k,x}u + L^h_{k,y}u - \frac{h_x^2}{12}L^h_{k,x}\frac{1}{p}L^h_{k,y}u - \frac{h_y^2}{12}L^h_{k,y}\frac{1}{q}L^h_{k,x}u =$$
$$= f - \frac{h_x^2}{12}L_{k,x}\frac{f}{p} - \frac{h_y^2}{12}L_{k,y}\frac{f}{q} + O(h^4).$$

Here $L^h_{k,x}$, $L^h_{k,y}$ are finite-difference one-dimensional operators of type

$$L^{(h)}_{k,x}u = [p^{(k)}_{i-1/2,j}(u_{i,j} - u_{i-1,j}) - p^{(k)}_{i+1/2,j}(u_{i+1,j} - u_{i,j})]/h_x^2,$$

and coefficients $p^{(k)}_{i+1/2,j}$, are defined under conditions

$$L^h_x u = L_x u - \frac{h_x^2}{12}L_x(\frac{1}{p}L_x u) + O(h^4).$$

which can be established by direct seria expansion of truncation error.

The generalization for 3D equation

$$Lu \equiv -\frac{\partial}{\partial x}p\frac{\partial u}{\partial x} - \frac{\partial}{\partial y}q\frac{\partial u}{\partial y} - \frac{\partial}{\partial z}r\frac{\partial u}{\partial z} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} + c\frac{\partial u}{\partial z} + æu = f.$$

are the following $O(h^4)$ order compact approximations:

$$L^h u_h \equiv L^h_x u_h + L^h_y u_h + L^h_z u_h - \frac{h_x^2}{12} L^h_x \frac{1}{p}(L^h_y + L^h_z)u_h -$$
$$-\frac{h_y^2}{12} L^h_y \frac{1}{q}(L^h_x + L^h_z)u_h - \frac{h_z^2}{12}\frac{1}{r}(L^h_x + L^h_y)u_h + æ u_h =$$
$$= f_h - \Big(\frac{h_x^2}{12} L^h_x \frac{1}{p} + \frac{h_y^2}{12} L^h_y \frac{1}{q} + \frac{h_z^2}{12} L^h_z \frac{1}{r}\Big)(f - æu)_h.$$

The separate consideration is made for the Poisson equation in cylindrical coordinates

$$L_r u + L_z u \equiv -\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial u}{\partial r} - \frac{\partial^2 u}{\partial z^2} = f(r,z)$$

including special $O(h^4)$ approximation at the axis, on the base of asymptotic representations of differential operators L_r and L_r^2 for $r \to 0$.

Similar approach is applied for nonstationary problems, described by 2D and 3D parabolic and hyperbolic equations

$$\frac{\partial u}{\partial t} = Lu + f, \quad \frac{\partial^2 u}{\partial t^2} = Lu + f,$$

under corresponded initial data, and approximations of the orders $O(\tau + h^4)$, $O(\tau^2 + h^4)$ are proposed.

The discretized algebraic systems are investigated in the sence of conditions for symmetricity, monotonicity and stability properties. The convergence and error estimates for numerical solutions are proved in the vector norms. The efficiency of suggested algorithms are demonstrated by the results of numerical experiments for the set of test problems.

Remark. Some compact finite volume (integro-balanced) approximations for 2D and 3D Poisson equations with piece-wise constant coefficients are considered in [1], [2].

References

1. V.P.Il'in. High order balanced approximations for Poisson equation.–Sib.Math., J., v. 37, 1, 1996, 151–169.

2. Ya.L.Gurieva, V.P.Il'in. On second order finite volume approximation for 3D mixed boundary value problems.–Bulletin NCC (NA), 7, 1996, 51–70.

Abstract for proposed talk at ICOSAHOM 98

Approximation of Compressible Navier-Stokes Flow via Discontinuous Galerkin Method with Time Splitting.

A method to approximate the Euler equations and the Navier-Stokes equations describing compressible flow is presented. The method is a multi-domain approximation, and a variational form of the equations is found by making use of the divergence theorem. The method is similar to that of the Discontinuous-Galerkin method of Cockburn and Shu, but the implementation is constructed through a spectral, multi-domain approach. The advective and diffusive operators are approximated through the use of an operator splitting technique.

The spatial discretization is found through a multi-domain method, and the computational domain is separated into subdomains that only overlap on their boundaries. Within each subdomain, the approximation is constructed as a linear combination of the Lagrange interpolants on the abscissa of the Legendre-Gauss quadrature.

The Navier-Stokes equations describing compressible flow are approximated through the use of a time splitting technique. The action of the advective terms and the diffusive terms are approximated in separate steps. This is done to simplify the manner in which the subdomain interfaces can be treated.

The spatial approximation is constructed through the use of a discontinuous Galerkin scheme. The spatial scheme is constructed through a variational form. The advective operator is constructed through the variational form and the boundary integrals are approximated by finding the state variables on the subdomain interfaces and then constructing the flux at the subdomain interface through an upwinding scheme. Here a van Leer flux is used.

The diffusive operator is constructed through a variational scheme. The time splitting examined here makes use of a second order Runga-Kutta scheme for both operators. The Runga-Kutta scheme makes use of the operator calculated at two different time-steps, a current and future step. The viscous flux at the current step is averaged and a penalty term is included, while the future time step is only averaged.

Results from numerical trials will be given for the approximation of both the Euler equations and the Navier-Stokes equations. Approximation of a

flow within an expanding nozzle and flow around a circular cylinder will be given for the Euler equations. Approximations for Burger's equations, a simple two dimensional, a linear advection-diffusion equation, and Navier-Stokes compressible flow around a circular cylinder will be given.

A Hierarchy of Non-Reflecting Boundary Conditions and Finite Elements

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One class of numerical methods to solve problems in unbounded domains is based on truncating the infinite domain via an artificial boundary $\mathcal{B}$ and applying some boundary condition on $\mathcal{B}$, which is called a Non-Reflecting Boundary Condition (NRBC) [1]. Here, a systematic way is developed to derive *optimal local approximate NRBCs* that are used in conjunction with the finite element method. This paper summarizes and extends our previous work reported in [2]–[5].

We consider the solution of the two-dimensional Laplace, Helmholtz and modified Helmholtz equations outside an obstacle and in a semi-infinite strip. In the proposed method, an artificial boundary $\mathcal{B}$ is first introduced, and the exact nonlocal Dirichlet-to-Neumann (DtN) boundary condition is derived on $\mathcal{B}$. This condition is then *localized*, and a two-parameter hierarchy of local NRBCs on $\mathcal{B}$, of increasing order, is obtained. The problem in the interior domain, with one of the NRBCs on $\mathcal{B}$, is solved using the finite element method.

The local NRBC is optimal in that it best approximates the exact nonlocal DtN boundary condition for C^∞ functions in the L_2 norm. The two parameters which characterize a specific NRBC in the hierarchy are the order of the NRBC, K, and the number of modes represented in it, N. Typically $N > K$, so that the optimal NRBC may represent modes of higher order than the order of the condition itself. We also consider the special case $N = K$, and show that this case leads to the localized DtN conditions derived in our previous work in a totally different manner.

The following issues are also addresses:

- The numerical stability of the scheme is discussed. It is shown that not all the NRBCs in the (K, N)-hierarchy are stable. Those that are stable are identified.
- A two-parameter hierarchy of special conforming finite elements is developed and used in the layer adjacent to $\mathcal{B}$, in conjunction with the local high-order NRBCs applied on $\mathcal{B}$. The two parameters are the required smoothness, which is related to K, and the order of interpolation p.
- An error analysis is given for the local NRBCs. More specifically, an error estimate is developed for the case of a positive operator, which depends on h (the mesh parameter), p, N and K. Numerical experiments are presented which validate the theoretical estimate.

In addition, the performance of the optimal NRBCs is demonstrated via numerical examples.

References

[1] D. Givoli, *Numerical Methods for Problems in Infinite Domains*, Elsevier, Amsterdam, 1992.

[2] I. Patlashenko and D. Givoli, "Nonlocal and Local Artificial Boundary Conditions for Two-dimensional Flow in an Infinite Channel," *Int. J. Numerical Methods for Heat and Fluid Flow*, 6, pp. 47–62, 1996.

[3] I. Patlashenko and D. Givoli, "Non-Reflecting Finite Element Schemes for Three-Dimensional Acoustic Waves," *J. Comput. Acoustics*, 5, pp. 95–115, 1997.

[4] D. Givoli, I. Patlashenko and J.B. Keller, "High Order Boundary Conditions and Finite Elements for Infinite Domains," *Comp. Meth. Appl. Mech. Engng.*, 143, pp. 13–39, 1997.

[5] D. Givoli and I. Patlashenko, "Optimal Local Non-Reflecting Boundary Conditions," *Applied Numerical Mathematics*, submitted.

From ENO to CWENO: High-Order Methods for Hyperbolic Systems of Conservation Laws

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We present a new family of high-order finite-difference methods for approximating solutions of hyperbolic systems of conservation laws

$$u_t + f(u)_x = 0, \quad u \in \mathbf{R}^d, d \geq 1. \tag{1}$$

These Godunov-type methods are based on combining methods which were developed in the context of *upwind* schemes (such as Harten's ENO [3], [4], WENO [6], [5]), with methods that were taken from the *central* framework (such as Lax-Friedrichs [2], Nessyahu-Tadmor [7]).

We extend these two approaches and hence we enjoy the recent advances in reconstructing high-order accurate, non-oscillatory interpolants in the upwind setup, while retaining the advantages of central methods (they do not require the solution of (approximate) Riemann problems and they don't involve characteristic variables).

A first step towards such a unified view was taken in [1]. There, a high-order central scheme based on a ENO reconstruction was derived. Here, we take another step forward by deriving methods based on a new centered version of the Weighted Essentially Non-Oscillatory (WENO) reconstruction of point-values from cell-averages presented in [6]. Our CWENO (Central-WENO) reconstruction is then utilized in the central framework to obtain a high-order, robust, essentially non-oscillatory method which is superior to our previous method in [1].

We explicitly construct the third and fourth-order scheme and demonstrate its high-resolution properties in several numerical tests.

Central schemes for conservation laws

To approximate solutions of (1), we introduce a mesh in the $x-t$ plane, the spatial grid-points are denoted by x_j. We denote by Δx and Δt, the spacing in the x and in the t variables respectively, and abbreviate by I_j the cell around x_j, i.e., $I_j := \left\{\xi \| \xi - x_j| \leq \frac{\Delta x}{2}\right\}$. By $w_j \sim u(x_j)$, we denote the approximate solution at x_j, and define $\bar{w}_j$ as the average of w_j over the cell I_j.

We introduce a piecewise-polynomial approximate solution at the discrete time levels. $t^n = n\Delta t$, based on the polynomials $R_j(x, t^n)$, were $\chi_j(x)$ denotes the characteristic function of the interval I_j,

$$w(x,t)|_{t=t^n} = \sum_j R_j(x,t^n)\chi_j(x), \quad \chi_j(x) := 1_{I_j}. \tag{2}$$

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Our reconstruction of the polynomials $R_j(x,t^n)$, which is the heart of the method, is based on a new Central-WENO reconstruction outlined below.

An *exact* evolution of w, based on integration of the conservation law over the staggered cell, $I_{j+\frac{1}{2}}$, then reads

$$\bar{w}_{j+\frac{1}{2}}^{n+1} = \frac{1}{\Delta x}\int_{I_{j+\frac{1}{2}}} w(x,t^n)dx - \frac{1}{\Delta x}\int_{\tau=t^n}^{t^{n+1}} [f(w(x_{j+1},\tau)) - f(w(x_j,\tau))]\,d\tau. \tag{3}$$

The first integral is the staggered cell-average at time t^n, $\bar{w}_{j+\frac{1}{2}}^n$, which can be computed directly from the above reconstruction. Due to the staggering, the time integrals of the flux are computed in smooth regions (up to a certain CFL condition) and hence, they can be approximated by any sufficiently accurate quadrature formula (e.g., for a fourth-order method one can use Simpsons rule). The required intermediate values required in the quadrature are predicted using either a Taylor expansion or a Runge-Kutta (RK) method which is more efficient (in particular for high-order methods for and systems). Our numerical scheme utilized a RK method with a natural continuous extension (taken from [8]) which requires only one step of the RK method from which the rest of the requires values can be reconstructed with the desired accuracy.

The CWENO reconstruction

Our new CWENO reconstruction is a modification of the reconstruction procedure suggested in [6]. There, in the so-called *Weighted Essentially Non-Oscillatory* (WENO) method, instead of selecting one stencil according to a non-oscillatory criterion, the interpolant is created by taking a convex combination of all candidate stencils. The weights of this combination are determined through a non-linear computation which is based on the local smoothness of the stencil. Every stencil is weighted according to the oscillations which it might create. In discontinuous regions, e.g., the weights will be biased towards the stencils in the smoother regions. Since, effectively, in smooth regions the linear combination of the different stencils can be interpreted as a wide stencil, a higher-order scheme can be constructed without using polynomials of a higher degree in the reconstruction procedure. An efficient implementation of WENO schemes and a new criterion for measuring the local smoothness of the stencils was presented in [5].

We derive a fourth-order reconstruction which results in a fourth-order method based on a polynomial of degree 2. Our interpolant takes the form

$$R_j(x) = \sum_{k=j-1}^{j+1} w_k^j P_k(x), \qquad \sum_{k=j-1}^{j+1} w_k^j = 1, \quad w_k^j \geq 0, \tag{4}$$

where $P_k(x)$ are polynomials reconstructed based on different stencils around x_j. The reconstructed polynomial $R_j(x)$ must satisfy conservation requirements ($\int_{I_j} R_j(x)dx = \Delta x \bar{u}_j$) and accuracy requirements (on the reconstruction of cell-averages, point-values and the derivatives of the flux). Additional non-oscillatory requirements (in the sense of ENO/WENO) enter through the choice of the weights w_k^j in (4). The above requirements take a different form in the central framework compared with their upwind form. This eventually amounts to a *new Central-WENO reconstruction* $R_j(x)$.

The reconstruction (4) is finally combined with the general central method (3) resulting with a new high-order, efficient and robust scheme.

References

[1] Bianco F., Puppo G., Russo G., SIAM J. Sci. Comp., to appear.

[2] Friedrichs K. O., Lax P. D., Proc. Nat. Acad. Sci., **68**, (1971), pp.1686-1688.

[3] Harten A., JCP, 49, (1983), pp.357-393.

[4] Harten A., Engquist B., Osher S., Chakravarthy S., JCP, **71**, (1987), pp.231-303.

[5] Jiang G.-S., Shu C.-W., JCP, **126**, (1996), pp.202-228.

[6] Liu X.-D., Osher S., Chan T., JCP, **115**, (1994), pp.200-212.

[7] Nessyahu H., Tadmor E., JCP, **87**, no. 2 (1990), pp.408-463.

[8] Zennaro M., Math. Comp., **46**, (1986), pp.119-133.

ICO98-32

Solution of Time Dependent Differential Equations with Variable Coefficients using Multidomain Legendre Method

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We present a new numerical algorithm for the solution of time dependent differential equations of the diffusion type. It allows for an accurate and efficient treatment of multidimensional problems with variable coefficients, nonlinearities and general boundary conditions.

The present algorithm incorporates several techniques. For the *space discretization* we use multidomain Legendre method. The computational region is decomposed into rectangular subdomains. Local problems are discretized using pseudospectral Legendre method.

For the *time discretization* we employ a new method proposed in [1]. A distinctive feature of this method is the exact evaluation of the contribution of the linear part (therefore, the corresponding schemes are labeled as "exact linear part" *(ELP) schemes*). As a result, this method has very good stability properties since possible instability may be due only to the nonlinear term. Typically, the stability of time-discretization schemes for advection-diffusion equations are controlled by the linear, diffusion, term and therefore these equations require implicit treatment in order to avoid the use of unreasonably small time steps. In contrast, using the explicit ELP scheme, it is possible to achieve stable time steps usually associated only with implicit schemes.

When a time dependent problem is solved using an explicit time inte-

gration scheme, boundary conditions should be imposed, and the values on boundaries have to be computed such that they satisfy the correct time dependent boundary conditions. In the present algorithm we adopt a *penalty procedure* of [2] to impose the *boundary conditions*. The penalty term is introduced as a forcing in the evolution equation. Its amplitude is proportional to the difference between the numerical and the prescribed boundary values. General boundary conditions (periodic, Dirichlet, Neumann, Robin) can be treated in this manner.

Coefficients of the ELP schemes have a form of exponential functions of elliptic operators with variable coefficients. Such global operators are typically represented by dense matrices. Therefore computing and applying exponentials of elliptic operators is expensive. In our paper we construct the global exponential operators in such a way the the interaction is confined within each subdomain. Here we employed a *generalized scaling and squaring method* for computing operator valued quadrature coefficients of the ELP schemes. In the matrix representation of the second derivative operator in the Legendre basis we discard the off-diagonal blocks which are responsible for the interaction with neighboring intervals. In effect, the matrices of global elliptic operators are obtained in a block diagonal structure with the block size equal to the order of local Legendre polynomials, k, and the number of blocks is equal to the number of subdomains, N

In order to restore the interaction between subdomains we developed a *penalty approach on the interfaces*, similar to that used on the boundaries. As a result, the complexity of the computational algorithm reduces drastically. For example, the operation count for evaluating in $d-$ dimensions (global) exponential functions of differential operators on the finest scale drops from $O(N^{3d}k^{3d})$ (when the interaction was incorporated into the operator) to the order of $O(N^d k^{3d})$ (when using block-diagonal matrices along with the penalty procedure on the interfaces). Thus, for a fixed order of Legendre polynomials, the computational complexity of the present algorithm is proportional to the number of subdomains.

Numerical results are presented for evolution equations with variable coefficients in one and two spatial dimensions.

References

[1] G. Beylkin, J.M. Keiser, L. Vozovoi, A new class of time discretization schemes for the solution of nonlinear PDEs, PAM Report No. 347, 1998, also submitted to J. Comput. Phys.

[2] J.S. Hesthaven, D. Gottlieb. A stable penalty method for the compressible Navier-Stokes equations. I. Open boundary conditions, *SIAM J. Scient. Comp.*, (1996), p.579-612.

Runge-Kutta Time Advancing for High Order Central Schemes

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We describe a technique to integrate hyperbolic systems of conservation laws with high accuracy, and using very little information on the structure of the particular system under consideration.=20

We integrate the following hyperbolic system of d equations:

$$u_t + f_x(u) = 3D0, \qquad u \in R^d,\ d \geq 1, \tag{1}$$

with a high order (3 or 4) central scheme. The integration in time must preserve the simplicity of the=20 underlying central scheme. We describe how to achieve this goal exploiting the Natural Continuous Extension (NCE) of Runge-Kutta schemes, studied in [8] and applied to the=20 integration of PDE's in [1].

Let k and h denote the time step and the spatial grid spacing respectively. Consider the grid $\{x_j\}$ defined at $t = 3Dt^n$ and let $I_j = 3D(x_j - h/2, x_j + h/2)$. In central schemes (see [7] and [6]), we integrate (1) form t^n to t^{n+1} on the staggered cells $(x_j, x_{j+1}) \times (t^n, t^{n+1})$.

Given the cell-averages $\bar{u}_j^n$ of the computed solution at time t^n, we first reconstruct the point values of u:

$$u(x, t^n) = 3D \sum_j R_j(x, t^n)\chi_j(x). \tag{2}$$

Here χ_j is the characteristic function of the cell I_j and R_j is a suitable polynomial defined on the $j-$th cell. This polynomial must be chosen in order to preserve high accuracy and to prevent the onset of spurious oscillations. In the present context, suitable choices are the Central ENO reconstruction of [1] or the CWENO reconstruction of [4]. These reconstructions are adapted from their upwind analogs. In particular, we refer to [2] for the ENO reconstruction and to=20 [5] and [3] for the WENO case.

The updated values of the cell averages on the steggered grid are obtained integrating (1) on the staggered cells:

$$\bar{u}_{j+1/2}^{n+1} = 3D\frac{1}{h}\int_{I_{j+1/2}} u(x, t^n)\,dx - \frac{1}{h}\int_0^k \left[f(u(x_{j+1}, t^n + \tau)) - f(u(x_j, t^n + \tau))\right]\,d\tau. \tag{3}$$

Since the solution $u(x, t^n + \tau)$ is smooth at x_j for τ small enough (more precisely, we need =20 $k \leq h/(2|a|)$, where a is the maximum characteristic speed), we can approximate the time integrals with a quadrature rule:

$$\int_0^k f(u(x_j, t^n + \tau))\,d\tau \simeq k \sum_l f(u(x_j, t^n + \tau_l))\,\omega_l,$$

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where τ_l and ω_l are the knots and weights of the quadrature formula (Simpson's rule is adequate for=20 methods of order up to 4).

We still need to predict u at the intermediate time levels $t^n + \tau_l$. This can be effectively done with Runge-Kutta schemes, solving the system of uncoupled ODE's:

$$\begin{cases} u_t(x_j, \cdot) = 3D - f_x(u(x_j, \cdot)) \\ u(x_j, t^n) = 3DR_j(x_j, t^n). \end{cases} \tag{4}$$

Using NCE's, we only need to evaluate u with one Runge-Kutta step at the final time t^{n+1}.

The NCE of a ν stage RK scheme is a collection of ν=20 polynomials of degree $d \leq \nu$. These polynomials are completely determined by the coefficients of the RK scheme. A suitable combination of these polynomials with the intermediate=20 values of the solution, obtained at each of the ν stages of the=20 RK scheme, provides a solution $O(k^d)$ accurate uniformly in=20 $[t^n, t^{n+1}]$. We use this solution to evaluate $u(x_j, t^n + \tau_l)$. Note that this technique results in a considerable saving of computational time, since, without NCE's, the RK scheme should be applied to each node of the quadrature formula.

The accurate evaluation of $f_x(u)$ is a key step in the time=20 marching scheme. It can be computed through high order non-oscillatory piecewise polynomial interpolations of the=20 point values of $f(u)$, as described in [1] or [4] in the Central ENO and the C-WENO context respectively.

Note that only the flux function f must be provided: no evaluation of the eigenvalues or eigenvectors of the Jacobian of f is necessary. The scheme can be applied componentwise to systems of equations, with no need to project along characteristic directions.

We show some numerical results obtained with third and fourth order schemes that illustrate the accuracy and the high resolution properties of our schemes.

References

[1] Bianco F., Puppo G., Russo G., SIAM J. Sci. Comp., to appear.

[2] Harten A., Engquist B., Osher S., Chakravarthy S., JCP, **71**, (1987), pp 231-303.

[3] Jiang G. S., Shu C. W., JCP, **126**, (1996), pp 202-228.

[4] Levy D., Puppo G., Russo G., preprint.

[5] Liu X. D., Osher S., Chan T., JCP **115**, (1994). pp 200-212.

[6] Liu X. D., Tadmor E., Numer. Math., to appear.

[7] Nessyahu H., Tadmor E., JCP, **87**, 2, (1990), pp 408-463.

[8] Zennaro M., Math. Comp., **46**, (1986), pp 119-133.

The errors in calculating the pseudospectral differentiation matrices for Čebyšev-Gauss-Lobatto points

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In the matrix version of pseudospectral methods one typically expands the approximate solution u_n as an interpolating polynomial in its Lagrangian form

$$u_n(x) := \sum_{k=0}^{n} u_n(x_k) L_k(x), \tag{1}$$

so that the unknown coefficients are directly the values of the corresponding function at the interpolation points. The $L_k(x)$ in (1) are the Lagrange polynomials. The Čebyšev pseudospectral method on $[-1,1]$ with boundary values uses the Čebyšev-Gauss-Lobatto points $x_k := \cos\frac{k\pi}{n}, k = 0(1)n$, as interpolation points. The derivatives of u_n can be estimated at the collocation points by differentiating (1) and evaluating the resulting expression. This yields

$$u_n^{(p)}(x_j) = \sum_{k=0}^{n} u_n(x_k) L_k^{(p)}(x_j), \qquad p = 1, 2, \ldots \tag{2}$$

or in matrix notation

$$\mathbf{u}^{(p)} = \mathbf{D}^{(p)}\mathbf{u}, \tag{3}$$

where

$$\mathbf{u} := [u_n(x_0), \ldots, u_n(x_n)]^T. \qquad \mathbf{u}^{(p)} := \left[u_n^{(p)}(x_0), \ldots, u_n^{(p)}(x_n)\right]^T, \tag{4}$$

and $\mathbf{D}^{(p)}$ is the $(n+1)\times(n+1)$ matrix whose entries are given by $D_{jk}^{(p)} := L_k^{(p)}(x_j), j, k = 0(1)n$. Such derivatives may be calculated analytically for $p = 1$ and 2.

As noted, e.g. by Breuer and Everson errors much larger than machine precision arise when calculating the matrix $\mathbf{D}^{(p)}$ for Čebyšev points. As a consequence, the errors in the first derivative computed as in (3) grow like n^4, dominating any n^2-inner-product accumulation error in $\mathbf{D}^{(1)}\mathbf{u}$.

In order to shed another light on the error, we suggest to consider the following relation among the entries of the differentiation matrices

$$L_j^{(p)}(x_j) = - \sum_{k=0,\ k\neq j}^{n} L_k^{(p)}(x_j) : \tag{5}$$

every diagonal element of the differentiation matrix should equal the negative sum of all other elements on its row. This reflects the fact that all the derivatives of constant functions vanish. This relation, together with the *barycentric representation* of the interpolating polynomial, lead to two novel ways of alleviating the errors:

- an algorithm of Schneider and Werner for computing the derivatives of the interpolating polynomial in its barycentric form;
- a formula of the same authors for the entries of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$.

Our experiments demonstrate that maintaining the relation (5) is more important than calculating certain elements of the differentiation matrix precisely, which results in the above algorithms being the most precise of all. It looks as if, as n increases, preventing $D_{00}^{(p)}$ and $D_{nn}^{(p)}$ from following the continuous deterioration of the other elements results in an "unbalanced" differentiation operator.

Modelling Convection Problem by Spectral Method with Chebyshev Basis Functions.

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The 3D penetrative convection problem is studied numerically by using the Fourier-Chebyshev spectral method. The vertical domain is infinite and is divided into three layers. In the middle layer, a negative temperature gradient is precsribed. Above and below the middle layer are two semi-infinite layers with positive temperature gradient. After a critical Rayleigh number is reached, fluid in the middle layer becomes unstable and convection motion penetrates into the stable layers.

There are several choices of basis functions in vertical direction. Recently, Tse & Chasnov have solved the problem successfully by using spectral method with the Hermite basis functions. Derivatives are carried out through transformation and semi-implicit time stepping scheme is used. However, Hermite functions cannot be employed if the variable does not decay to zero or the decay rate not exponential. This occur for the mean quantities and special treatment for them are required.

To improve the situation, the Hermite basis functions are now replaced by Chebyshev polynomials with algebraic mapping. The polynomials are renamed as Rational Chebyshev Polynomials and their properties are studied by J.P. Boyd. In this work, derivatives are carried out through matrix multiplications. Since the mapping has relaxed the time-stepping constraint imposed by collocation points near the boundary, explicit scheme becomes feasible.

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Several LES simulations are carried out with resolution of 64^3 and 128^3 up to Rayleigh number of 1×10^6. The second order and third order moments are studied. The asymptotic decay rate at high Rayleigh number is different for the stable and unstable region. The values match with results obtained from analytic derivation. Furthermore, the relative advantages of using Hermite and Chebyshev method will be compared.

Fast and High-Order Solutions to the Spherical Shallow Water Equations

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Many current state-of-the-art global atmosphere models utilize the spectral transform method (STM). This class of methods provides an elegant solution to the pole problems induced by a spherical coordinate system. Waves are uniformly resolved at all points on the sphere including the poles, and the resulting stability and accuracy have made it the method of choice for most models. The major drawbacks of the method are its computational cost and communication overhead on parallel processors. If N represents the number of latitude points on the surface of the sphere, the associated Legendre transforms of the STM require $\mathcal{O}(N^3)$ operations, which is larger than any other computation in weather modeling by a factor of N. At the time the STM rose in popularity, it was competitive at the resolutions contemporary computing architectures could handle, and for smooth fields is still the cheapest method per digit of accuracy. However, to resolve certain small-scale atmospheric features, N has been increased to the point that the Legendre transforms require a significant portion of the overall computing time.

Since its adoption in global climate models, the hope has been that a fast Legendre transform would be found, in the sense of the fast Fourier transform. This would provide computations in spherical geometry with the efficiency available in Cartesian geometry, but this goal has not been realized. Here we develop a class of fast spherical shallow water equation solvers using methods that reduce or bypass the explicit computations of Legendre transforms. Our search has been guided by the following observations:

1. Spherical harmonics provide an isotropic representation of functions on the surface of the sphere. Although unstructured grid methods can produce nearly-isotropic solutions, they are unlikely to be incorporated into existing weather models because of the underlying grid structure. On the other hand, latitude-longitude grids, which are highly non-isotropic, have some advantages in terms of ease of storage and periodicity, but introduce a set of problems associated with the poles. For example, the grid spacing near the poles places an unacceptable restriction on the time step. For this reason, methods based on latitude-longitude grids use filtering to maintain stability. Filtering is also used to dealias the nonlinear terms.

2. A number of fast methods for computing spatial derivatives on latitude-longitude grids already exist which have been largely ignored due to the popularity of the STM. These approaches warrant re-examination with new filters, in conjunction with lessons learned from our current models, and in the context of the now-standard shallow water test suite [1]. These methods include the pseudospectral approach of Merilees [2, ?] (recently revived by Fornberg [4]) and the fourth-order compact approach of Gilliland [5]. Our findings strongly suggest that the difference between spectral and fourth-order accuracy is negligible for realistic problems if a suitable filter is applied.

3. A nearly ideal filter exists. The spherical harmonic filter (SHF) is obtained if we transform the variables to spherical harmonic space and directly back to grid space thus projecting our approximations onto the space of spherical harmonic basis functions. Since there are fewer harmonics than grid points, this results in a truncation of non-isotropic waves. For Merilees' method for computing spatial derivatives filtered with the SHF, the results are *identical* to the STM (within machine precision) while requiring fewer transforms than the most efficient STM. The SHF is not a fast algorithm in the sense of the FFT or finite difference operators. However, Jakob and Alpert [6] have recently published a fast multipole SHF (which was subsequently improved by Yarvin and Rokhlin [7]). Combined with a fast method for computing spatial derivatives, this implies the existence of a fast STM in the sense of a fast Fourier transform.

References

[1] D. L. Williamson, J. B. Drake, J. J. Hack, R. Jakob, and P. N. Swarztrauber. A standard test set for numerical approximations to the shallow water equations in spherical geometry. *Journal of Computational Physics*, 102(1):211–224, September 1992.

[2] Philip E. Merilees. Numerical experiments with the pseudospectral method in spherical coordinates. *Atmosphere*, 12(3):77–96, 1974.

[3] Philip E. Merilees. The pseudospectral approximation applied to the shallow water equations on the sphere. *Atmosphere*, 11(1):13–20, 1973.

[4] Bengt Fornberg. A pseudospectral approach for polar and spherical geometries. *SIAM Journal on Scientific Computing*, 16(5):1071–1081, September 1995.

[5] Ronald L. Gilliland. Solutions of the shallow water equations on the sphere. *Journal of Computational Physics*, 43(1):79–94, 1981.

[6] Rüdiger Jakob-Chien and Bradley K. Alpert. A fast spherical filter with uniform resolution. *Journal of Computational Physics*, 136:580–584, 1997.

[7] Norman Yarvin and Vladimir. Rokhlin. A generalized one-dimensional fast multipole method with application to filtering of spherical harmonics. Technical Report Research Report 1142, Yale Computer Science Department, 1998.

Enhanced shock detection in spectral viscosity approximations of nonlinear conservation laws

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ABSTRACT

In this paper we construct, analyze and implement a new procedure for edge detections in the context of spectral approximations for nonlinear conservation laws.

It is well known that using spectral methods for nonlinear conservation laws will result in the formation of the Gibbs phenomenon once spontaneous shock discontinuities appear in the solution. These spurious oscillations will in turn lead to loss of resolution and render the standard spectral approximations unstable.

The Spectral Viscosity (SV) method [Tadmor] was developed to stabilize the spectral method by adding a spectrally small amount of high-frequencies diffusion carried out in the dual space. The resulting (SV) approximation is stable without sacrificing spectral accuracy.

The (SV) method recovers a spectrally accurate approximation to the *projection* of the entropy solution, but the projection is at best a first order approximation to the exact solution as a result of the formation of the shock discontinuities.

The issue of spectral ***resolution*** is addressed by post-processing the (SV) solution to remove the spurious oscillations at the discontinuities, as well as increase the $O(\frac{1}{N})$ accuracy away from the shock discontinuities. Successful post-processing methods have been developed to eliminate the Gibbs phenomenon and recover spectral accuracy for the (SV) approximation. However, such reconstruction methods require apriori knowledge of the locations of the shock discontinuities. Therefore, the detection of these discontinuities is essential to obtain an overall spectrally accurate solution. To this end, we employ the recently constructed *enhanced edge detectors* based on appropriate concentration factors [Gelb, Tadmor]. Once the edges of these discontinuities are identified, we can utilize a post-processing reconstruction method, and show that the post-processed (SV) solution recovers the exact entropy solution with remarkably high-resolution.

We consider two numerical examples:

1. The one-dimensional inviscid Burgers' equation with periodic boundary conditions. This is a good test case as the solution admits a nonstationary shock discontinuity originating at a critical spatial and temporal value.

2. The one-dimensional system of the Euler equations of gas dynamics, subject to different initial conditions.

We apply the Fourier and Chebyshev (SV) methods to the one-dimensional inviscid Burgers' equation, and the Chebyshev (SV) method to the one-dimensional system of gas dynamics. We then employ the enhanced edge detectors to locate the shock discontinuities. Finally we utilize a spectrally accurate post-processing method [Gottlieb, Shu, et. al.] based on the Gegenbauer polynomials to obtain a highly accurate approximation to the entropy solution.

Large time step Godunov–type schemes for Hamilton–Jacobi equations

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We consider high–order approximations to Hamilton–Jacobi equations of the form

$$\begin{cases} v_t + H(x, \nabla v) = 0 \\ v(x,0) = v_0(x) \end{cases}$$

with $H(x,\cdot)$ convex. The integral Bellman representation formula for the solutions allows to built a class of schemes of the Godunov type, which do not suffer from the usual limitation on the CFL number. The general structure of such schemes is a discretization of the representation formula in the form:

$$\begin{cases} v_j^n = \min_\alpha \left[\Delta t \Phi_2(x_j, \alpha, \Delta t) + I[V^{n-1}](x_j + \Delta t \Phi_1(x_j, \alpha, \Delta t))\right] \\ v_j^0 = v_0(x_j). \end{cases}$$

The particular structure of a scheme derives from the choice of Φ_1, Φ_2 (which are supposed to be discretizations of Runge–Kutta type for a suitable system of ODEs describing characteristics), and of the reconstruction operator $I[V^{n-1}]$ (of linear, monotone or ENO type).

We present some concrete examples of schemes of this class characterized by a high order of consistency, with a stability analysis for some of them. We also discuss the qualitative behaviour (monotonicity, resolution of discontinuities,...) and the influence of the discretization parameters on the efficiency of the schemes. Limitations of this approach are also discussed.

Lastly, numerical examples in $\mathbb{R}^1$ and $\mathbb{R}^2$ for equations of eikonal type are presented.

References

[1] M. Falcone and R. Ferretti, Discrete–time high–order schemes for viscosity solutions of Hamilton–Jacobi–Bellman equations, Num. Math. **67** (1994), 315-344.

[2] M. Falcone and R. Ferretti, Convergence analysis for a class of semi–lagrangian advection schemes, SIAM J. Num. Anal., **35** (1998), to appear.

[3] A. Harten, On a large time–step high resolution scheme, Math. Comp. **46** (1986).

[4] R. J. LeVeque, A large time step generalization of Godunov's method for systems of conservation laws, SIAM J. Num. Anal., **22** (1985).

[5] S. Osher and C. W. Shu, High–order essentially non–oscillatory schemes for Hamilton–Jacobi equations, SIAM J. Num. Anal., **28** (1991), 907–922.

Bounded-Error Finite Difference Schemes for Initial Boundary Value Problems on Complex Domains

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Abstract

Bounded error scheme are a schemes in which the error norm is bounded by a function of the time t, the mesh size h and the exact solution to the differential problem u (typically a Sobolev norm of u), i.e. $\| \epsilon \| < F(u,h,t)$, $F < \infty \; \forall \; t < \infty$, where $F \to 0$ as $h \to 0$. In practice we use the error boundness in a stricter sense. We require that $\| \epsilon \|$, the L_2 norm of ϵ, be bounded by a "constant" proportional to h^m (m being the spatial order of accuracy) for all $t < \infty$, or at most grow linearly in time, the time coefficient being proportional to h^m.

A methodology for constructing finite-difference semi-discrete schemes, for initial boundary value problems (IBVP), on complex, multi-dimensional shapes is presented. This method has as its starting point the construction of one dimensional schemes on a uniform grid with boundary points that do not necessarily coincide with the extremal nodes of the mesh. The boundary conditions are imposed using simultaneous approximation terms (SAT). The 1-D schemes are built in a way that the the coefficient matrix of the corresponding ODE system which represents the error evolution in time is negative definite (N.D.) and bounded away from 0 by a constant independent of the size of the matrix, or is at least non-positive definite (N.P.D.). These properties, N.D. or N.P.D., enable us to prove that the scheme is error-bounded by a "constant", or error-bounded by linear growth in time, respectively. Since a sum of two negative (non-positive) definite matrices is a negative (non-positive) definite matrix, a multi-dimensional scheme can be built by adding differentiation operators each of which is negative (non-positive) definite.

This methodology was used to develop second and fourth order accurate approximations for $\partial^2/\partial x^2$ and a second order accurate approximation for $\partial/\partial x$. Using these approximations error-bounded schemes were constructed for the one and multi-dimensional diffusion and linear advection-diffusion equations. Numerical examples show that the method is effective even where standard schemes, stable by traditional definitions, fail.

The methodology was adopted to construct error-bounded schemes for parabolic equations and systems containing mix-derivatives and for the wave equation $u_{tt} = \nabla^2 u$.

Explicit v.s. Implicit Time Integration Schemes in Conjunction with a Modified Fourier Method

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When traditional finite difference or finite element methods are applied to the space discretization of advection-diffusion equations, it is well-known that certain implicit-explicit (IMEX) schemes normally represent the most efficient schemes for the time integration [1]. Explicit time integration schemes are also often prohibitively expensive for such equations if the space discretization is performed by traditional Legendre or Chebychev spectral methods, since such methods involve non-uniform grids resulting in severe restrictions on the timesteps [2], [6].

In this work we shall demonstrate that explicit time integration schemes are competitive, and often even preferable, when we perform space discretization for the advection-diffusion equation in one dimension by the modified Fourier collocation method developed in [3], [4]. The main reasons for this are that this method utilizes a uniform grid and has very good resolution properties.

The modified Fourier collocation method enables us to handle nonperiodic problems by utilizing piece-wise Bernoulli polynomials in addition to the trigonometric functions. The method is a generalization of the idea of polynomial subtraction considered earlier by various authors [6], [8], [9], [10]. The key difference in this method compared to the usual Fourier method is that we at each timestep have to accurately calculate the spatial derivatives of as many orders as possible of the solution at the boundary points. Accurate equations for these derivatives are established in [3], [4], and additional equations will be given for the problem under consideration here. Utilizing these equations, an accurate numerical method of high order is established for the advection-diffusion equation with nonperiodic boundary conditions. Numerical calculations confirming the theoretical estimates regarding the accuracy will be given, and the excellent resolution properties of the method will be demonstrated.

Emphasis will be laid on comparing explicit time integration schemes with IMEX schemes for both advection and diffusion dominated equations. Since

the employed grid is uniform, we can expect that the stability limit when using explicit time integrating schemes will be much more favourable than the $O(N^{-4})$ limit for traditional Legendre or Chebyshev spectral methods. Indeed, this was confirmed in [5] where the modified Fourier collocation method was applied to the heat equation in one- and two- dimensions, in simple as well as in complex geometries. Using a (4)5th order explicit Runge-Kutta scheme, DOPRI5 [7], for the time integration, we find that the stability limits for the time steps for the advection-diffusion equation are similar to those obtained in [5] for the heat equation.

As is well-known, the difference between the time steps giving stability and those giving maximal accuracy is quite small for high order explicit schemes like DOPRI5. For implicit and IMEX schemes, however, the stability time steps will usually be much larger than the time steps providing maximal accuracy. By choosing different specified accuracies, we determine the time steps necessary to reach these accuracies for both well resolved and poorly resolved solutions. The time steps provided by DOPRI5 are compared to the corresponding time steps when using several IMEX schemes from [1] for the time integration.

It will be shown that in cases where we have much structure per gridpoint, the explicit scheme is not only competitive compared to the IMEX schemes, but is in fact clearly preferable, and that this holds even for diffusion dominated equations. Since our aim is to extend the methods to realistic 3D problems where we normally only can expect marginal resolution of the solutions, this is a very promising result. In fact, explicit time integration schemes are much more attractive with respect to implementation on parallel computers, the potential for the modified Fourier collocation method therefore looks very good indeed.

References

[1] U. M. Ascher, S. J. Ruuth and B. T. R. Wetton, Implicit-explicit methods for time-dependent partial differential equations, *SIAM J. Numer. Anal.*, **32**, (1995), pp. 797–823.

[2] C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang, *Spectral Methods in Fluid Dynamics*, Springer-Verlag, New York, NY, (1988).

[3] K. S. Eckhoff, On a high order numerical method for solving partial differential equations in complex geometries. *J. Scientific Comp.* **12** (1997), pp. 119–138.

[4] K. S. Eckhoff, On a high order numerical method for functions with singularities. To appear in *Math. Comp.* (1998).

[5] K. S. Eckhoff and C. E. Wasberg, *Solution of parabolic partial differential equations in complex geometries by a modified Fourier collocation method.* Proc. 3. Internat. Conf. Spectral and High Order Methods, ICOSAHOM'95 (Houston, Texas, U.S.A., 1995), edited by A.V. Ilin and L.R. Scott (Houston Journal of Mathematics, 1996), pp. 83–91.

[6] D. Gottlieb and S. A. Orszag, *Numerical Analysis of Spectral Methods: Theory and Applications,* CBMS-NSF Regional Conference Series in Applied Mathematics **26**, Society for Industrial and Applied Mathematics, Philadelphia, PA, (1977).

[7] E. Hairer and S. P. Nørsett and G. Wanner", *Solving ordinary differential equations I, nonstiff problems*, Springer-Verlag", Berlin, (1987).

[8] C. Lanczos, *Discourse on Fourier Series*, Oliver & Boyd, Edinburgh, (1966).

[9] J. N. Lyness, *Computational techniques based on the Lanczos representation.* Math. Comp. **28**, (1974), pp. 81–123.

[10] P. J. Roache, A pseudo-spectral FFT technique for nonperiodic problems, *J. Comp. Phys.*,**27**, (1978), pp. 204-220.

Fourth Order Accurate Compact Implicit Method for the Maxwell Equations

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Abstract

We consider a fourth order accurate compact scheme for the numerical solution of the Maxwell equations. We use the same mesh stencil as used in the standard Yee scheme. In particular extra information over a wider stencil is not required. This has several advantages. First, it is relatively easy to modify an existing code based on the Yee algorithm to make it fourth order accurate. Second, a staggered mesh, without additional mesh locations, makes the boundary treatment easier since some of the quantities are located inside the domain rather than on the boundary. Finally, a staggered grid system gives a lower error than a similar non-staggered system.

We base this scheme on the following relation:

$$\begin{bmatrix} 26 & -5 & 4 & -1 & . & . & 0 \\ 1 & 22 & 1 & 0 & . & . & 0 \\ 0 & 1 & 22 & 1 & 0 & . & 0 \\ . & . & . & . & & & \\ 0 & . & . & 0 & 1 & 22 & 1 \\ 0 & . & . & -1 & 4 & -5 & 26 \end{bmatrix} \frac{\partial}{\partial x} \begin{bmatrix} U^{1/2} \\ U^{3/2} \\ . \\ . \\ U^{(2p-1)/2} \end{bmatrix} = \frac{24}{\Delta x} \left(\begin{bmatrix} U^1 \\ U^2 \\ . \\ U^{p-1} \\ U^p \end{bmatrix} - \begin{bmatrix} U^0 \\ U^1 \\ . \\ U^{p-2} \\ U^{p-1} \end{bmatrix} \right).$$

The error in the fourth order scheme decreases significantly with comparison to Yee's second order scheme. This allows us to use a much coarser mesh, and therefore use less computer time.

We present numerical results not only for simple cases as waveguides and sources in free space, but also for dielectrics. We smooth the dielectric coefficients with a fourth order implicit interpolation. This interpolation reduces the errors, both for the Yee scheme and the fourth order scheme. In the new scheme the error decreases dramatically. This enables us to use a coarser mesh and less computer time in comparison to Yee's scheme.

We conclude that the fourth order scheme is more accurate and efficient than Yee's scheme. Yee's scheme requires a mesh about 8 times finer in each direction than the fourth order scheme to achieve similar accuracy and hence requires much more computer time for the same accuracy.

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Toward the Construction of Fourth-Order Difference Scheme for Complex Domains in Cartesian Grid

E. Turkel and A. Yefet

Abstract

We consider fourth order accurate compact schemes for numerical solutions to the Maxwell equations. We base this scheme on Ty(2,4) scheme([?]). This scheme uses a cartesian grid for all domains. As in Yee's and Ty(2,4) schemes, we use a staggered mesh for the approximation of the spatial derivatives and for the time derivatives we use the leapfrog scheme. We begin with Maxwell equations in one dimension:

$$\begin{aligned} \frac{\partial E_z}{\partial \tau} &= Z\frac{\partial H_y}{\partial x} \\ \frac{\partial H_y}{\partial \tau} &= \frac{1}{Z}\frac{\partial E_z}{\partial x} \end{aligned}$$

Where $Z = \sqrt{\frac{\mu}{\epsilon}}$, ϵ and μ are the permittivity and permeability coefficients, in free space.

Instead of using $HY_{\frac{1}{2}}$ we use $HY_{\frac{\gamma}{2}}$ where $\gamma\Delta x$ is the distence between EZ_1 and the first point EZ_γ.

We Define:

$$\hat{M} = \begin{bmatrix} a_l & 0 & . & . & . & . & 0 \\ a_{l1} & b_{l1} & c_{l1} & 0 & . & . & 0 \\ 0 & 1 & 22 & 1 & 0 & . & 0 \\ . & . & . & . & & & \\ 0 & . & 0 & 1 & 22 & 1 & 0 \\ 0 & . & . & 0 & c_{r1} & b_{r1} & a_{r1} \\ 0 & . & . & . & . & 0 & a_r \end{bmatrix}$$

And

$$\hat{N} = \begin{bmatrix} A_l & B_l & C_l & . & . & . & 0 \\ 1 & 22 & 1 & 0 & . & . & 0 \\ 0 & 1 & 22 & 1 & 0 & . & 0 \\ . & . & . & . & & & \\ 0 & . & 0 & 1 & 22 & 1 & 0 \\ 0 & . & . & 0 & 1 & 22 & 1 \\ 0 & . & . & . & C_r & B_r & A_r \end{bmatrix}$$

Where:

$$\begin{aligned} a_l &= 24\gamma_l \\ a_{l1} &= \frac{8}{(1+\gamma_l)(3+\gamma_l)} \\ b_{l1} &= \frac{4(5+6\gamma_l)}{(1+\gamma_l)} \end{aligned}$$

$$
\begin{aligned}
c_{l1} &= \frac{4}{(3+\gamma_l)} \\
A_l &= \frac{\gamma_l^3 + 9\gamma_l^2 + 24\gamma_l + 40}{2} \\
B_l &= -\gamma_l^3 - 6\gamma_l^2 + 5 \\
C_l &= \frac{\gamma^3 + 3\gamma_l^2 - 2}{2}
\end{aligned}
$$

For the right hand side we use the same coefficients but we use γ_r instead of γ_l.

The matrix form of these approximations is:

$$
\hat{M}\frac{\partial}{\partial x}\begin{bmatrix} EZ^{\gamma_l/2} \\ EZ^{3/2} \\ . \\ . \\ EZ^{p-\gamma_r/2} \end{bmatrix} = \frac{24}{\Delta x}\left(\begin{bmatrix} EZ^1 \\ EZ^2 \\ . \\ EZ^{p-1} \\ EZ^p \end{bmatrix} - \begin{bmatrix} EZ^{\gamma_l} \\ EZ^1 \\ . \\ EZ^{p-2} \\ EZ^{p-1} \end{bmatrix}\right).
$$

$$
\hat{N}\frac{\partial}{\partial x}\begin{bmatrix} HY^1 \\ HY^2 \\ . \\ . \\ HY^{p-1} \end{bmatrix} = \frac{24}{\Delta x}\left(\begin{bmatrix} HY^{3/2} \\ HY^{5/2} \\ . \\ HY^{p-3/2} \\ HY^{p-\gamma_r/2} \end{bmatrix} - \begin{bmatrix} HY^{\gamma_l/2} \\ HY^{3/2} \\ . \\ HY^{p-5/2} \\ HY^{p-3/2} \end{bmatrix}\right).
$$

We base this approximation on the following relations:

$$
\begin{aligned}
\frac{EZ_1 - EZ_\gamma}{\Delta x} &= a_l EZ_{\frac{\gamma}{2}x} + O(\Delta x^2) \\
\frac{EZ_2 - EZ_1}{\Delta x} &= a_{l1} EZ_{\frac{\gamma}{2}x} + b_{l1} EZ_{\frac{3}{2}x} + c_{l1} EZ_{\frac{5}{2}} + O(\Delta x^4) \\
\frac{HY_{\frac{3}{2}} - HY_{\frac{\gamma}{2}}}{\Delta x} &= A_l HY_{1x} + B_l HY_{2x} + C_l HY_{3x} + O(\Delta x^3)
\end{aligned}
$$

The construction of the two dimensional case is straightforward.

This scheme gives very good results, but it has two major drawbacks:

1. adjusting this scheme to three dimesions.
2. If γ is very small $\hat{M}$ becomes almost singular.

References

[1] E. Turkel and A. Yefet, "Fourth Order Accurate Compact Implicit Method for the Maxwell Equations," to appear.

How to make the three-point scheme exponentially convergent

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We show that a special distribution of grid steps of the standard three-point finite-difference (FD) approximation of a two-point linear operator problem increases from second to exponential (even superexponential for some cases) the convergence order of the Neumann-to-Dirichlet map (ND). We relate the approximate ND to a rational function and calculate FD steps using the Padé-Chebyshev approximation of the impedance function of the continuous problem.

Let us consider the two-point problem on $[0, L]$, $L > 0$ (including $L = +\infty$)

$$Aw(x) - \frac{d^2w(x)}{dx^2} = 0, \qquad \left.\frac{dw}{dx}\right|_{x=0} = -\varphi,\ w(L) = 0. \tag{1}$$

Here we for simplicity assume that φ and $w(x)$ are respectively vector and vector-function in a Hilbert space, A is a x-independent self-adjoint positive-definite bounded operator, however all the results will be valid for unbounded operators provided the spectrum of the Neumann data is bounded. The ND can be defined as $w(0) = f(A)\varphi$, through the impedance function $f(\lambda) = \frac{1-e^{-2L\sqrt{\lambda}}}{\sqrt{\lambda}(1+e^{-2L\sqrt{\lambda}})}$.

The FD solution is defined at "potential" nodes x_i, $i = 1, \ldots, k+1$, $x_1 = 0$, $x_{i+1} > x_i$, the FD derivatives are defined at nodes $\hat{x}_i$, $i = 0, \ldots, k$, $\hat{x}_0 = 0$. We denote $h_i = x_{i+1} - x_i$, $\hat{h}_i = \hat{x}_i - \hat{x}_{i-1}$ and allow both h_i and

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$\hat{h}_i$ to be arbitrary positive numbers to increase the degree of freedom for the optimization. Instead of (1) we will solve the FD problem

$$Aw_i - \frac{1}{\hat{h}_i}\left(\frac{w_{i+1}-w_i}{h_i} - \frac{w_i - w_{i-1}}{h_{i-1}}\right) = 0, \qquad i = 2, \ldots, k,$$

$$Aw_1 - \frac{1}{\hat{h}_1}\left(\frac{w_2 - w_1}{h_1}\right) = \frac{1}{\hat{h}_1}\varphi, \qquad w_{k+1} = 0. \tag{2}$$

The crucial fact is that $w_1 = f_k(A)\varphi$, where the discrete impedance function $f_k(\lambda)$ is a rational function of λ depending on $h_i, \hat{h}_i$ as parameters. We will optimize the error of computing the ND using (2), i.e., minimize the bound $\delta_k = \|w(0) - w_1\| \leq \max_{\lambda\in[\lambda_{min},\lambda_{max}]} |f_k(\lambda) - f(\lambda)|\,\|\varphi\|$, where $\lambda_{min} = \|A^{-1}\|$ and $\lambda_{max} = \|A\|$. So we arrived at the problem of the rational approximation of f by f_k on $[\lambda_{min}, \lambda_{max}]$. Let θ_i and s_i be respectively the eigenvalues and the first components of the corresponding eigenvectors of the finite-difference operator (2), then $f_k(\lambda) = \sum_{i=1}^{k} \frac{s_i^2}{\lambda - \theta_i}$. The Padé–Chebyshev approximant $f_k(\lambda)$ on $[\lambda_1, \lambda_2]$ is defined by the conditions

$$\int_{\lambda_1}^{\lambda_2} \lambda^i \left[f_k(\lambda) - f(\lambda)\right] \rho(\lambda)\, d\lambda = 0, \qquad i = 0, 1, \ldots, 2k-1, \tag{3}$$

where $\rho(\lambda)$ is the Chebyshev spectral weight adjusted to $[\lambda_1, \lambda_2]$. Intuitively, the best choice for $[\lambda_1, \lambda_2]$ would be $[\lambda_{min}, \lambda_{max}]$. However, for large quotients $\lambda_{max}/\lambda_{min}$ better convergence of δ_k is obtained if $\lambda_1 = \lambda_{min}$, $\lambda_2 \approx 4\lambda_{min}^{1/3}\lambda_{max}^{2/3}$.

If $L = +\infty$, the spectrum is continuous, and we can obtain the exponential convergence $\delta_k \cong O\left[\exp\left(-4k\sqrt[6]{\frac{\lambda_{min}}{\lambda_{max}}}\right)\right]$.

If $L < +\infty$ the spectral measure is discrete. The logarithmical capacity of the discrete spectrum is equal to 0 and we arrive at the *superexponential* convergence!

Algorithm of calculation of $h_i, \hat{h}_i$:

1°. Find $s_1, \ldots, s_k, \theta_1, \ldots, \theta_k$ from (3).

2°. Solve the inverse spectral problem, i.e., from θ_i and s_i obtain h_i and $\hat{h}_i$, $i = 1, \ldots k$.

We demonstrate numerical examples exhibiting the exponential convergence for a semiinfinite domain and the superexponential convergence for a bounded domain, then show an extension to hyperbolic equations (indefinite A).

Multidomain Pseudospectral Computation of Maxwell's Equations in 3-D General Curvilinear Coordinates

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Abstract

In this paper, we discuss numerical solution of 3-D Maxwell's equations in general curvilinear coordinates. The numerical scheme we use is a multidomain pseudospectral (Chebyshev collocation) scheme, and the absorbing boundary condition we use to truncate the computational domain is the perfectly matched layer (PML) method.

In our multidomain approach, we decompose complex computational domains into simple subdomains that can be mapped onto a hexahedral. In each subdomain we apply the usual Chebyshev collocation method. To facilitate the application of the PML method, we generate multi-layers of subdomains to surround 3-D objects. The perfectly matched layer is put in the out-most layer of subdomains. By putting the PML's in a separate layer of subdomains, we avoid any problem of approximating non-smooth solutions, across vacuum-layer interface, with high-order polynomials.

For perfect electrical conducting (PEC) objects, the inner domain of the object is not computed. Instead, PEC boundary condition is applied on the object surface for the scattered field being computed. For dielectric and lossy dielectric objects, however, we also need to simulate the inner domain of the objects. A total field/scattered field formulation is used in the simulation for excitation.

The PML method we use is strongly well-posed. In fact, the modified Maxwell's equations we need to solve for the method are symmetric hyperbolic. The rectangular PML method, the cylindrical PML method, or the spherical PML method is applied in the simulation of different problems.

We apply the characteristic relations in patching solutions on subdomain interfaces. Due to the fact that normal vector is not well defined at edges and corners, we does not patch the solutions simultaneously. Instead, we apply the patching conditions in multiple sweeps of the subdomain interface, and the solutions on the subdomain interface are patched perfectly after all sweeps are done, i.e. solutions belong to different subdomains are equal on common subdomain interfaces.

On subdomain interfaces that are also (lossy) dielectric object surface, we apply appropriate patching conditions, different from the characteristic-type conditions, that are consistent with the physical conditions at the surface. Our approach is found to be stable and accurate in numerical experiments.

In the numerical experiments, we simulate scattering by a cube, a sphere, and a cylinder. We consider PEC, dielectric, and lossy dielectric materials. We compare our results with the Mie-series analytical results for spheres and other numerical results.

which shows the high-order accuracy of our computation. The use of spectral methods, especially multidomain spectral methods, appears to be very promising in accurate simulation of electromagnetic wave problems.

NUMERICAL SIMULATION OF INCOMPRESSIBLE FLOWS IN ENCLOSED CYLINDER(S) USING A SPECTRAL PROJECTION METHOD

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The understanding of transition to turbulence in rotating systems requires a fundamental knowledge of the vortical waves present on the axis, in the endwall and sidewall boundary layers, and in free shear layers in the interior inclined at arbitrary angles to the rotation axis, and the interactions and couplings between them. A complicating property of rotating flows is that distant boundaries may be surprisingly important (when compared to situations in non-rotating flows). One cannot automatically suppose that, so long as the size of the system is large compared to the length scale of the shearing region, one is dealing with an effectively infinite expanse of fluid. Hence, it is important to take into account the endwall effects when dealing with strong rotating flows. However, the endwalls introduce an additional level of numerical difficulties when compared to the axial-periodic case.

To simplify the presentation, we shall present the scheme for the axisymmetric case. The scheme can be readily extended to fully three-dimensional cases by using the Fourier expansion for the azimuthal direction. We denote

$$\mathcal{D} = \{(r,z) : r \in (r_i, r_o) \text{ and } z \in (0,\Lambda)\}, \quad \tilde{\nabla} = \partial_r^2 + \frac{1}{r}\partial_r + \partial_z^2, \tag{1}$$

$$\tilde{\Delta} = \begin{pmatrix} \tilde{\nabla}^2 - 1/r^2, & 0, & 0 \\ 0, & \tilde{\nabla}^2 - 1/r^2, & 0 \\ 0, & 0, & \tilde{\nabla}^2 \end{pmatrix}, \quad \tilde{\nabla} = \begin{pmatrix} \partial_r \\ 0 \\ \partial_z \end{pmatrix}, \tag{2}$$

where r_i and r_o are respectively the radius of the inner ($r_i = 0$ if only one cylinder is present) and outer cylinder, Λ is the height of the cylinder(s). Then, the Navier-Stokes equations in cylindrical coordinates can be written as

$$\begin{aligned} &\boldsymbol{u}_t - \frac{1}{Re}\tilde{\Delta}\boldsymbol{u} + \tilde{\nabla}p + N(\boldsymbol{u}) = 0, \\ &\tilde{\nabla}\cdot\boldsymbol{u} := \frac{1}{r}(ru)_r + w_z = 0, \end{aligned} \tag{3}$$

subjected to appropriate boundary conditions

$$B(t)\boldsymbol{u}|_{\partial\mathcal{D}} = 0,$$

where $\boldsymbol{u} = (u, v, w)^T$ and $N(\boldsymbol{u})$ is the vector containing the nonlinear terms.

To overcome the difficulties associated with the nonlinearity and the coupling between the velocity components and the pressure, we use the following semi-implicit second-order projection scheme (cf. [6, 3]):

$$\begin{aligned} &\frac{1}{2\delta t}(3\tilde{u}^{k+1} - 4u^k + u^{k-1}) - \frac{1}{Re}\tilde{\Delta}\tilde{u}^{k+1} = -\tilde{\nabla}p^k - (2N(u^k) - N(u^{k-1})), \\ &B(t^{k+1})\tilde{u}^{k+1}|_{\partial\mathcal{D}} = 0, \end{aligned} \tag{4}$$

$$
\begin{aligned}
&-\tilde{\nabla}^2(p^{k+1}-p^k) = -\frac{1}{2\delta t}\tilde{\nabla}\cdot\tilde{\boldsymbol{u}}^{k+1},\\
&\frac{\partial}{\partial \boldsymbol{n}}(p^{k+1}-p^k)|_{\partial\mathcal{D}} = 0,
\end{aligned}
\tag{5}
$$

and

$$
\boldsymbol{u}^{k+1} = \tilde{\boldsymbol{u}}^{k+1} - 2\delta t\tilde{\nabla}(p^{k+1}-p^k). \tag{6}
$$

where δt is the time step, $\tilde{\boldsymbol{u}}^{k+1} = (\tilde{u}^{k+1}, \tilde{v}^{k+1}, \tilde{w}^{k+1})^T$ and $\boldsymbol{u}^{k+1} = (u^{k+1}, v^{k+1}, w^{k+1})^T$ are respectively the intermediate and final approximations of $\boldsymbol{u}$ at time $t^{k+1} = (k+1)\delta t$.

Hence, at each time step, we only have to solve a vector Helmholtz equation for $\tilde{\boldsymbol{u}}^{k+1}$ and a Poisson equation for p^{k+1}. We use a new, fast spectral-Galerkin method (cf. [4]) with which Helmholtz/Poisson equations in enclosed cylinder(s) can be solved with spectral accuracy and quasi-optimal computational complexity, despite the presence of non-constant coefficients and coordinate singularity (in case $r_i = 0$). The combination of the second-order semi-implicit projection scheme and the spectral-Galerkin method results in a very efficient and accurate algorithm for simulating unsteady incompressible flows in enclosed cylinder(s).

Rotating flows in enclosed cylinder(s) often involve discontinuous (Dirichlet) boundary conditions which will result in unwanted oscillations and contaminate the accuracy of the spectral method. We have developed a sensible strategy to approximate discontinuous boundary conditions to within any prescribed accuracy by using smooth boundary layer functions so that spectral method can still be safely applied to problems with discontinuous boundary conditions.

The above scheme is used to simulate a number of canonical rotating flows, including:

- **Endwall boundary layer flow:** We consider the impulsive spin-down of a fluid in solid body rotation within a circular cylinder (cf. [2]). This flow leads to rapid development of thin boundary layers whose nature and stability are strongly influenced by the rotation.
- **Parametrically forced Taylor-Couette flow:** We consider the Taylor-Couette flow with real endwall effects and harmonic oscillations of the inner cylinder in the axial direction. Previous studies (cf. [5, 1]) have shown that the onset of centrifugal instabilities (Taylor cells) can be controlled by parametric excitation through the harmonic axial motion of the inner cylinder.

We shall present a detailed investigation of these canonical flows in an effort to isolate generic mechanisms which lead to transitions to turbulence in rotating flows and to design corresponding dynamic control mechanisms to either delay transition or limit the intensity of the resultant instabilities.

This is a joint work with John Lopez.

REFERENCES

[1] K. T. Coughlin and P. S. Marcus. Modulated waves in Taylor–Couette flow. Part 2. Numerical simulation. *J. Fluid Mech.*, 234:19–46, 1992.

[2] J. M. Lopez and P. D. Weidman. Stability of stationary endwall boundary layers during spin-down. *J. Fluid Mech.*, 326:373–398, 1996.

[3] Jie Shen. On error estimates of projection methods for the Navier-Stokes equations: second-order schemes. *Math. Comp*, 65:1039–1065, 1996.

[4] Jie Shen. Efficient spectral-Galerkin methods III. polar and cylindrical geometries. *SIAM J. Sci. Comput*, 18:1583–1604, 1997.

[5] S. J. Tavener, T. Mullin, and K. A. Cliffe. Novel bifurcation phenomena in a rotating annulus. *J. Fluid Mech.*, 229:483–497, 1991.

[6] J. van Kan. A second-order accurate pressure-correction scheme for viscous incompressible flow. *SIAM J. Sci. Stat. Comput.*, 7:870–891, 1986.

Spatial development of wakes using a spectral multi-domain method

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In order to solve the Navier-Stokes equations in geometries of large aspect ratio, a spectral multi-domain method has been recently proposed [1]. The resulting solver has already been used for the solution of the thermohaline convection equations [2], within the Boussinesq approximation. It is now adapted to the computation of wakes in stratified fluids. In the present paper we briefly summarize the numerical technique and mainly focus on some crucial points, directly connected with the considered physical problem, namely the spatial development of wakes in fluids stably stratified by a thermal gradient.

The multi-domain technique is implemented along the direction of great length, in order to enable the treatment of geometries of large aspect ratio. In each subdomain the incompressible Navier-Stokes equations are solved by using a $P_N - P_N$ Chebyshev collocation method, yielding a divergence-free velocity field. The matching conditions between the subdomains are the classical interface conditions, but the one involving the pressure is only enforced weakly, in order to overcome the difficulty arising from the so-called "spurious modes" of pressure. An influence matrix technique is used to enforce these matching conditions and, at the interfaces of the sub-domains, the velocity components are expressed in appropriate bases, chosen to be fully consistent with (i) the boundary conditions and (ii) the incompressibility constraint. Moreover, the pressure field can be accurately recovered, if necessary, despite the use of the $P_N - P_N$ approximation.

The non-linear convective term is splitted, in order to take into account implicitly the part associated with the mean flow velocity. This leads us to use an advection-diffusion operator, whose mathematical properties will be analyzed. The problem of the outflow boundary conditions, which is much more delicate with high-order methods than with low-order's, will be considered. Especially, the results obtained with the commonly used outflow conditions, which essentially consist in calculating the velocity components at the boundary from an advection equation involving the mean flow velocity, will be discussed and compared to other approaches yielding a better efficiency, in terms of accuracy and stability.

Finally, the abilities of the method will be illustrated with some numerical experiments concerning the spatial development of wakes in stratified fluids, downstream a velocity profile of Bickley type. The results show the influence of the stratification on the unsteady flows obtained for different values of the Richardson and Reynolds numbers.

1. C. Sabbah, R. Pasquetti, A divergence-free multi-domain spectral solver of the Navier-Stokes equations in geometries of high aspect ratio, to appear in the Journal of Computational Physics.

2. C. Sabbah, R. Peyret, R. Pasquetti, On the double diffusive instability of a stratified fluid subject to lateral heating, Conf. Instabilities in stratified and / or rotating flows, Moscou, 24-27 june 1997.

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NUMERICAL STUDY OF STABILITY, BIFURCATIONS AND SLIGHTLY SUPERCRITICAL STATES OF CONFINED FLOWS USING A GLOBAL GALERKIN METHOD

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The present study is devoted to the analysis of the linear stability of numerically calculated fluid flows and the weakly nonlinear analysis of their slightly supercritical states. The problem of linear stability of a steady flow leads to an eigenvalue problem. If the steady flow is calculated numerically, the size of the eigenvalue problem is equal to the number of degrees of freedom of the numerical method, i.e., number of discretization nodes multiplied by number of unknown scalar functions. The solution of an eigenvalue problem of such large size is rarely possible. Necessity to reduce the number of degrees of freedom leads to higher-order methods. For canonical domains (domains whose boundaries are coordinate surfaces) a spectral method with globally defined basis functions can be efficiently applied.

The present work is devoted to the application of the Galerkin method with globally defined basis functions to the analysis of stability of numerically calculated steady flows. The basis functions are built with the help of computer algebra as linear superpositions of Chebyshev polynomials in such a way that they satisfy analytically all the boundary conditions and the continuity equation [1,2]. Several test calculations which show the possibility of reducing the number of degrees of freedom without reduction of accuracy are reported.

The described numerical approach is applied to several problems: stability of swirling flow in a cylinder with independently rotating top and bottom [2,3], stability of free-buoyancy convection in laterally heated cavities [1,4], and axisymmetry-breaking bifurcations of axisymmetric convective flows [5]. The results are verified by a numerical solution of the same problems using a second-order finite volume method which plays the role of numerical experiment.

A possibility to reduce the number of degrees of freedom is shown in Fig.1, where a steady flow in a cylinder with rotating lid is calculated by the Galerkin and the finite volume methods. The illustrated swirling flow contains three recirculation vortex bubbles. Comparison with the experimental photo [6] shows that all three bubbles are resolved correctly with the use of 34×34 basis functions of the Galerkin method and with a 200×200 stretched finite volume grid. At the same time the upper recirculation region is resolved inaccurately with a 100×100 grid.

An example, shown in Fig.2, illustrates an axisymmetry breaking instability of convective flow in a cylinder. In the experiments of Kowalewski [7] the sidewall and the bottom of the cylinder were maintained at a hot temperature, while the top was maintained at a cold temperature. At a certain temperature difference the axisymmetric flow bifurcates to an asymmetric one, which contains 16-18 azimuthally distributed flow structures. An experimental photo of the distribution of the temperature below the cold top is shown in Fig.2a. The numerical analysis of stability of this flow was based on the assumption that the resulting 3D flow has 8- or 9-fold symmetry. The calculated *most unstable perturbation* of the temperature is shown in Fig.2b. The isolines of the perturbation are plotted at the same axial cross section where the temperature isolines shown in Fig.2a were photographed. It is seen that the pattern of the calculated perturbation of the temperature and the experimental photo are similar.

Stability diagrams for different swirling and convective flows and the corresponding slightly supercritical oscillatory flow states will be reported at the conference.

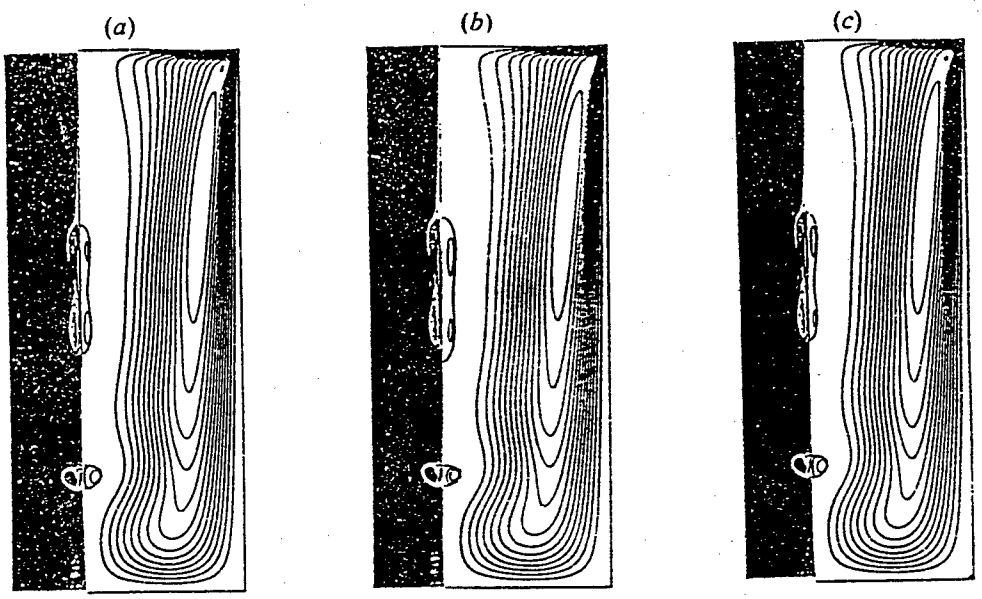

Fig.1. Meridional flow streamlines in a cylinder with rotating lid. Re=2752, aspect ratio 3.25. Comparison with the experimental result of Escudier (1984). (a) Calculation with the Galerkin method using 34×34 basis functions. (b) Calculation with the finite volume method using the 100×100 stretched grid. (c) Calculation with the finite volume method using the 200×200 stretched grid.

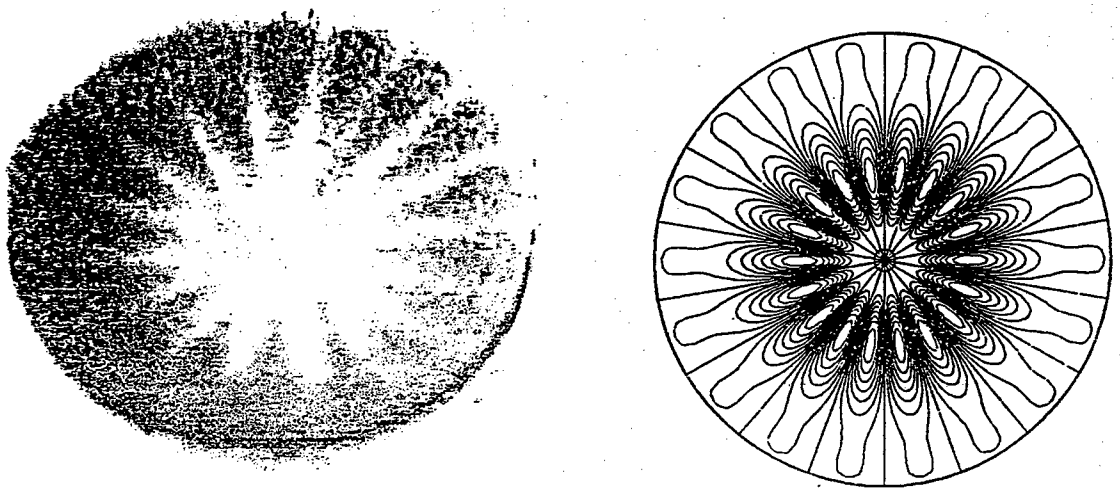

Fig.2. Axisymmetry-breaking instability of a convective flow in a cylinder. (a) Exprimental photo of the temperature distribution below the cold cover. (b) Isolines of the calculated 3D perturbation of the temperature in the axial cross section below the cold cover.

References

1. Gelfgat A.Yu. and Tanasawa I. 1994. Numerical analysis of oscillatory instability of buoyancy convection with the Galerkin spectral method. *Numerical Heat Transfer. Part A: Applications*, 25(6), 627-648.
2. Gelfgat A., Bar-Yoseph P. and Solan A. 1996. Stability of confined swirling flow with and without vortex breakdown. *Journal of Fluid Mechanics*, 311, 1-36.
3. Gelfgat A., Bar-Yoseph P. and Solan A. 1996. Vortex breakdown and instability of swirling flow in a cylinder with rotating top and bottom. *Physics of Fluids*, 8(10), 2614-2625.
4. Gelfgat A., Bar-Yoseph P. and Yarin A. 1997. On oscillatory instability of convective flows at low Prandtl number (to appear in *Journal of Fluids Engineering*)
5. Gelfgat A., Bar-Yoseph P. and Solan A. 1997. Axisymmetry-breaking instabilities of axially symmetric convective flows. *Proc. 10th Int. Conf. on Transport Phenomena in Thermal Science and Process Engineering*. Kyoto, December 1-4, 1997, Vol.1, pp.263-268.
6. Escudier M.P. 1984. Observation of the flow produced in a cylindrical container by a rotating endwall. *Exps. Fluids* 2, 189-196.
7. Kowalewski T. *Private communication*.

A fully distributed parallel solver for multidimensional Helmholtz/Schroedinger equations

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A fully distributed - in operations and memory - parallel solver for multidimensional Helmholtz/Schroedinger equations is presented. The solver is based on a parallel preconditioner which is derived from the generic structure of the Helmholtz/Schroedinger partial differential equations with scattering boundary conditions. At the heart of the algorithm is a new novel parallel preconditioner for the linear system as

$$\left(\sum_{l=1}^{N}(\mathcal{A}_l+\alpha_l\mathbf{I}_l)-(\mathcal{V}+\alpha\mathbf{I})\right)\chi=\phi, \qquad \left(\sum_{l=1}^{N}\mathcal{A}'_l-\mathcal{V}\right)\chi==\phi. \qquad (1)$$

The parallel preconditioner is based on an explicit formula for the inverse of the separable part of $\mathcal{A}$, i.e.,

$$\mathcal{G}=\left(\sum_{l=1}^{N}\mathcal{A}'_l\right)^{-1}.$$

$$\varphi=\mathcal{G}\phi=(\prod_{l=n}^{1}\mathcal{W}_l^{-1})\mathcal{D}^{-1}(\prod_{l=1}^{n}\mathcal{U}_l^{-1})\phi,$$

where we compute the spectral decomposition of $\mathcal{A}'_l=\mathcal{U}_l\mathcal{D}_l\mathcal{W}_l$ as in [2].

The efficient parallel implementation of the preconditioner is made available through the design of a special multidimensional matrix vector product algorithm. We envision the vector ϕ of order $N=\Pi_{l=1}^{n}N_l$, as a multidimensional cube of order n, with sides N_l. We similarly envision the system of parallel processors as a cube machine of order n, with sides P_l, where

$\Pi_{l=1}^{n} P_l = P$ is the number of processors in the system. We can then distribute the vector ϕ equally among the cube processors, letting each store a corresponding sub block of order $M = \Pi_{l=1}^{n} M_l, M_l = N_l/P_l$, and apply the product independently in each direction. We thereby reduce the communication overhead considerably. For example, for $P_l = P/n$, by a factor of $P/\log(P)$, with respect to the standard multiplication algorithm.

As an application we consider an electron wave in a rectangular electron wave guide ("quantum wire") in which the electron motion is quantized along the lateral (x, y) directions. Along the propagation (z) direction the free electrons are scattered over a barrier associated with an abrupt change of the Fermi energy[1]. The computational speedup is demonstrated in fig.1 for up to 64 processors on a distributed memory IBM SP2. The three dimensional $(n = 3)$ wavefunction was distributed into to sub blocks of size $20 \times 20 \times 40$, where the number of blocks was determined by the number of available processors, $P = 1 - 64$.

=2.in F1.eps =2.in F2.eps

Figure 1: A plot of the electron probability density $|\chi(x, y, z)|^2$ in the (x, z) plane inside the waveguide, $(y = 0)$ illustrating the transmission and reflection due to scattering. 442368 grid points were used to sample the wave function ($N_x = 48$, $N_y = 48$, $N_z = 192$) and 20 operations of $\mathcal{G}$ were required for obtaining the solution to the desired accuracy. The Flops vs. processors, illustrating the linear speedup is depicted on the right.

References

[1] U. Peskin, W. H. Miller and Å. Edlund, Quantum time-evolution in time-dependent fields and time-independent reactive-scattering calculations via an efficient Fourier grid preconditioner, J. Chem. Phys. **103**, 10030 (1995). preconditioner, J. Comput. Phys. 138 (1997).

[2] I. Bar-On and Victor Ryaboy, Fast Diagonalization of Large and Dense Complex Symmetric Matrices, with Applications to Quantum Reaction Dynamics, SIAM J. of Scientific and Stat. Comp., 28, 5, (1997).

An object-oriented toolbox for spectral element programming

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Spectral element methods are known to be quite demanding as far as programming effort is concerned. With respect to finite elements, spectral elements feature more involved element-level computations, like tensor products or grid-to-grid reinterpolations; polynomial or geometrical nonconformities, which can often be avoided in finite element implementation, bring about severe additional programming complexity. In order to come up with a reasonably easily maintanable implementation, one should thus rather resort to a high-level programming approach. The most popular candidate is object-oriented programming.

This talk describes Speculoos, a C++ program for spectral and mortar element analysis of partial-differential equations, whose design is grounded on object-oriented techniques. The expected benefit, in terms of understandability, ease of debugging, reusability and extendibility, over a standard unstructured procedural code typically implemented in Fortran 77 relies on a sound application of the object-oriented programming concepts, mainly data encapsulation.

The program consists in a library of classes, which are introduced now. Four element classes describe 0D to 3D spectral elements: Vertex, Edge, Face, Volume. Elements are usually regrouped into objects of class Mesh. On a mesh the user can define a number of objects of type Field, e.g., a coordinate field, pressure fields, velocity fields, temperature fields. A flexible mechanism allows Legendre-family interpolation to vary from direction to direction and from element to element, naturally supporting P_N-P_{N-K} formulations of any type ($0 \leq K \leq N$) and polynomial nonconformities. Fields are the cornerstone of Speculoos, because they are not only flexible data structures containing interpolation information and nodal values, but also active entities, able to perform a broad set of user-relevant operations: basic arithmetic operations such as saxpy-like summations, computations of Euclidian norm or grid-to-grid reinterpolations, differential operations such as evalutations of a weak gradient operator or a H1 norm, solving operations such as direct-stiffness assembly with mortar constraints, etc. These functions typically feature no more than 0 to 3 arguments, which make them easy to use. A programming environment is obtained by implementing, besides class Field, a number of analysis tools: classes DirichletCondition, LinearSolver, TimeIntegrationScheme (and subclasses such as Adams-Bashforth or BDF). Finally a set of common differential equations are regrouped as : classes Helmholtz, SteadyStokes, NavierStokes, etc.

In order to solve a problem, the user proceeds by creating an application in the so-called "main" program. In this application he/she creates objects and sends messages to these. A typical set-up of an application is the following: first, the user creates objects describing the problem geometry: elements and meshes; next the user creates a number of fields, with adequate interpolation, then boundary-condition and linear-solver objects; then the user assigns initial values to some fields, creates a problem object, assigns the aforementioned components to that problem, and requests from that problem to compute its solution; finally the user performs some error computations or sets up plots. Note that there is absolutely no requirement on what the application should consist in: there is no such programming constraints as an input file or a mandatory sequence of operations. Speculoos is not a classical-sense program, it is a class library; the application behaves as an empty sheet of paper the user fills according to his/her needs.

Besides creating applications, the user can also act as a programmer, by modifying or enriching the set of classes and their associated operations. Syntactically, creating an application or modifying the class library are identical tasks: both consist in creating objects and sending messages to them. There is no filter, such as command language, between the application level and the library level: both abide by the same, object-oriented, logic and by the same syntax, that of the implementation language.

Preliminary efficiency measurements are satisfactory. Although object-oriented programming naturally induces some time penalty over lower-level procedural programming, and although C++ compilers are not as optimized as Fortran analogues, execution times are competitive since most CPU time is ordinarily spent in tensor-product functions which rely on calls to BLAS routines. Also, the element-by-element implementation of the fields promotes a very degree of locality. Parallelizing Speculoos thus turned out to be straightforward.

Object-oriented programming proves to be an attractive approach for developing research program in numerical methods, even in computationally intensive areas such as spectral element methods.

A new Fekete point triangular spectral element method

Mark Taylor[1] and B. A. Wingate[2]

The spectral finite element method is a very straightforward way to implement a spectrally accurate algorithm while maintaining the use of fully unstructured grids. In this method, the computational domain is first broken up into rectangular regions called elements, and within each of these elements all variables are approximated by high degree polynomial expansions. The discrete equations are then derived using an integral form of the equations to be solved in conjunction with a clever choice of test functions and collocation points. As is well known, if conforming elements are used the resulting mass matrix is diagonal. This simple form of the method is perhaps the most natural way to achieve high order finite element methods. Its exponential convergence has been shown for realistic problems with many elements and polynomial degree as high as 56.

We are concerned with the simplest form of the spectral element method: conforming elements used to solve initial value problems such as the primitive equations. In this form, the method leads to a fully explicit, spectrally convergent method. This simple method is useful in real problems: it is currently used in the global three-dimensional ocean (SEOM [5]) and atmospheric (SEAM [8]) models. At present, this simple form of the spectral element method is only available with conforming quadrilateral grids. This is because the spectral element method relies on the existence of high order quadrature formulas which use the same number of collocation points as basis functions. For the square, these methods use a tensor product of Gauss-Lobatto collocation points.

Unfortunately, conforming quadrilateral grids can be quite complicated to generate. There are now automated programs to perform this task, but the grids are rarely as uniform as triangulations. More uniform grids can be constructed if one uses the mortar element approach, but then we lose the simple, fully explicit spectral element formulation.

The most natural alternative to this grid generation problem would be a triangular spectral element method. The most popular approach for high

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degree triangles has been that of [4, 7, 9]. The quadrature formula used in these spectral element methods is based on a warped tensor product grid. Unfortunately, this quadrature formula is over-sampled: it has more grid points than we have basis functions, making it impossible to construct basis functions which lead to a diagonal mass matrix. Nor does this approach have a particularly easy-to-invert mass matrix.

To develop a triangle based spectral element method with a diagonal mass matrix, we need to find an accurate set of collocation/quadrature points for the triangle where the number of points is the same as the number of basis functions. Constructing Gaussian quality quadrature formulas for the triangle turns out to be an extremely hard problem. Only few low degree special cases are known, and there are also several truncations for which it is known that Gaussian quadrature formulas do not exist. Gaussian (and Gauss-Lobatto) type quadrature formulas seem to be extremely rare, and restricted to a few simple domains like the 1D interval and its tensor products.

This leads us to propose a different derivation of the spectral element method, which we will base on the Fekete points rather than Gauss-Lobatto quadrature points. Many of the theoretical results known for the distribution of Fekete points can be found in [1]. As far as we know, the only works in which Fekete points have been computed are [2, 6, 3].

Fekete points are attractive for spectral element methods for several reasons. The definition of Fekete points is closely related to the expression for the associated cardinal functions (Lagrange interpolating functions) which are used as basis functions in spectral element methods. This in turn leads to cardinal functions which have well behaved approximation, quadrature and derivative properties. In the square, numerical evidence strongly suggests the Fekete points are the same as the Gauss-Lobatto points, and thus a Fekete point spectral element method is the same as the standard spectral element method. But unlike the Gauss-Lobatto points, the Fekete points are defined for any domain and with any polynomial truncation. Finally, Bos has conjectured that in the triangle the Fekete points on the boundary will be the one dimensional Gauss-Lobatto points. We have verified this conjecture numerically. This result has an important implication: Fekete point triangular elements will conform with standard quadrilateral spectral elements.

The only difficulty in using Fekete points seems to be computing them for large degree. In the triangle, they have been approximated by Bos [2] for up to degree 7. More recently, Chen and Babuška [3] improved and extended

these results to degree 13. They also computed L^2 norm optimal interpolation points, and showed that these points have a lower Lebesgue constant than their approximate Fekete points. We will present a new algorithm for computing Fekete points which allows us to extend these previous results to degree 19. Furthermore, for degrees larger than 11, our approximate Fekete points have lower Lebesgue constant than the L^2 optimal points computed in [3].

References

[1] T. Bloom, L. Bos, C. Christensen and N. Levenberg, *Polynomial interpolation of holomorphic functions in C and C^n,* Rocky Mountain J. Math., **22**, pp 441–470 (1992).

[2] L. Bos, *Bounding the Lebesgue function for Lagrange interpolation in a simplex,* J. Approx. Theory, **38**, pp 43–59 (1983).

[3] Q. Chen and Ivo Babuška *Approximate optimal points for polynomial interpolation of real functions in an interval and in a triangle,* Comput. Methods Appl. Mech. engrg. **128** pp 405–417 (1995).

[4] M. Dubiner, *Spectral methods on triangles and other domains,* J. Sci. Comp., **6** pp 345–390 (1993).

[5] D. Haidvogel, E. Curchitser, M. Iskandarani, R. Hughes and M. Taylor, *Global modeling of the ocean and atmosphere using the spectral element method,* Atmosphere-Ocean **35** (1997) 505–531.

[6] M. Reimer and B. Sündermann *A Remez-type algorithm for the calculation of extremal fundamental systems for polynomial spaces on the sphere,* Computing, **37** pp. 43–58 (1986).

[7] S. J. Sherwin and G.E. Karniadakis, *A triangular spectral element method; applications to the incompressible Navier-Stokes equations,* Comp. Meth. Appl. Mech. Eng., **123** pp. 189–229 (1995).

[8] M. Taylor, R. Loft, J. Tribbia. *Performance of a spectral element atmospheric model (SEAM) on the HP Exemplar SPP2000,* NCAR/TN-439+EDD.

[9] B. Wingate and J. P. Boyd, *Triangular spectral element methods for geophysical fluid dynamics applications,* Proceedings of the Third International Converence on Spectral and High Order Methods, Houston Texas, pp. 305–314 (1995).

The natural function space for the triangle and tetrahedra

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The success of the classical formulation of the spectral element method lies in the choice of functional space, grid points, and method of integration. On the quadrilateral, the prefered space is a tensor product basis of Legendre polynomials,

$$\mathcal{P}^2_\square = \{span(x^n y^m) | 0 \leq m \leq N; 0 \leq n \leq N\}. \quad (1)$$

The grid points are chosen as the Gauss-Lobatto-Legendre points, which lead to an accurate, well-behaved interpolation, and subsequently well-behaved derivatives. The choice of points is also important for coupling elements together easily. By choosing a quadrature slightly less accurate than the optimal Gaussian, one achieves a computationally efficient diagonal global mass matrix for explicit methods.

Despite this efficiency, there are several drawbacks to the quadrilaterals method. First, grid generation is more difficult for quadrilaterals than triangles, especially for solution adaptive methods. Second, it is known that quadrilaterals can give degenerate algorithms if the elements are too skewed. This motivates interest in finding an efficient spectral element method with triangular subdomains. Investigators who have proposed new algorithms for spectral elements on triangles include [2], [3], and [1]. In particular, Dubiner introduced a new orthogonal basis on the triangle, a warped product of Jacobi polynomials in the space,

$$\mathcal{P}^2_\triangle = \{span(x^n y^m) | 0 < m, n; m + n \leq N\}. \quad (2)$$

This is also the favorite approximation space for the finite element method. Dubiner defined this basis and outlined how to implement the method for trianglular subdomains. The Dubiner method has been successfully applied to the incompressible Navier-Stokes equations by Sherwin and Karniadakis [4], the shallow water equations by Wingate [6], and extended to three dimensional tetrahedra by Sherwin and Karniadakis [5]. While the method is stable, with eigenvalues for the first and second derivative matrices which are no worse than the quadrilaterals, it is complicated to implement. There is an advantage to using this method for the incompressible Navier-Stokes equations because the semi-implicit formulation is no more expensive to solve than the explicit method, and the global stiffness matrix is sparse. The efficiency of this approach has been extensively optimized and studied by Karniadakis and his collaborators.

While this basis is a generalized tensor product, the method as outlined by Dubiner does not have a well-behaved set of Cardinal functions. To couple elements

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together with C_0 continuity one must sacrifice some orthogonality, which makes the stiffness matrix non-diagonal for explicit methods. This is much more expensive than for the cleverly implemented explicit method on quadrilaterals. For atmospheric and oceanic simulations the loss of the diagonal global stiffness matrix is significant because there is little advantage to using a semi-implicit method for the diffusion terms because the maximum time step is limited by the speed of the free-surface gravity wave, not by the diffusion.

In this work we introduce a new spectral element method on triangles. Like the method on quadrilaterals it gives a diagonal mass matrix for explicit methods. It uses the Fekete points to form well-behaved Cardinal functions on the triangle. These points have been known since at least 1923, and depend on the choice of space. We will also present a new algorithm for computing these points.

In this work we ask the question, what is the natural functional space for triangles? We first observe that the space of functions usually used for the triangle and quadrilateral are different. Equation 1 represents a diamond truncation of polynomials while equation 2 is a triangle truncation. The basis functions on quadrilaterals are a tensor product of one-dimensional eigenfunctions of singular Sturm-Liouville problems and subsequently their convergence depends on the regularity of the function being approximated and no special conditions at element boundaries. Here we present, for the first time, the analogous singular Sturm-Liouville problem for the triangle and tetrahedron. We first pose a problem for the triangle which is invarient under the symmetry group, $D3$. Remarkably, the eigenfunctions of this problem are the Dubiner polynomials, $g_{m,n}(x,y)$. We show that the eigenvalues are $(m+n)(m+n+2)$, in contrast to those for the quadrilateral which are $m(m+1)+n(n+1)$. The eigenvalues validate the choice of triangular truncation, while the singular Sturm-Liouville problem guarantees good convergence properties for analytic functions. This problem is generalized to the N-dimensional simplex, introducing a new class of singular Sturm-Liouville problems.

We use this space and basis to compute the Fekete points and for doing operations in spectral space, such as filtering.

References

[1] M. Dubiner. Spectral methods on triangles and other domains. *J. Sci. Comp.*, 6:345–390, 1991.

[2] D. Funaro. Pseudospectral approximation of a pde defined on a triangle. *Applied Math. and Comp.*, 42:121–138, 1991.

[3] C. Mavriplis and John Van Rosendale. Triangular spectral elements for incompressible fluid flow. ICASE Report 93-100, 1993.

[4] S.J. Sherwin. and G.E. Karniadakis A triangular spectral element method; applications to the incompressible navier-stokes equations. *Comp. Meth. Appl. Mech. and Engr.*, 123:189–229, 1995.

[5] S.J. Sherwin. and G.E. Karniadakis Tetrahedra *hp* finite elements, algorithms and flow simulations. *J. Comp. Phys.*, 124:14–45, 1996.

[6] B.A.Wingate. *Spectral Elements using Triangular Subdomains for Geophysical Fluid Dynamics Applications.* PhD thesis, University of Michigan, 1996.

High Order Vorticity–Velocity Method for the Simulation of Pipe Flow Transition

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We introduce a numerical method which has been developed for investigations into the spatial transition from laminar to turbulent pipe flow.

It is based on a vorticity–velocity formulation of the Navier–Stokes equations in cylindrical co-ordinates for an incompressible fluid. We use 8th order compact finite differences in the radial and streamwise directions and a Fourier–spectral discretisation in the azimuthal direction.

The vorticity transport equation is integrated with respect to time employing a 4th order Runge–Kutta scheme. Combining such an explicit scheme with the angular over–resolution of the grid near the centre line would severely restrict the maximum time step. We, therefore, analytically integrate the r and ϕ derivatives of the viscous terms in order to obtain a system which is considerably less stiff. In addition, a high order filter stabilizes the integration.

There are no immediate physical boundary conditions for two of the three vorticity components. Yet such conditions can be derived from the requirement that both the vorticity and the velocity fields must be solenoidal. An influence matrix method has been implemented to calculate the proper values of the vorticity at the wall. Boundary conditions on the centre line are obtained from the symmetry of the co-ordinate system and by requesting that the angular dependence of the quantities and of their derivatives must vanish as $r \to 0$.

A direct Poisson solver based on a fast Fourier transform in the axial direction efficiently calculates the velocity corresponding to the vorticity.

A damping zone prevents the numerical outflow boundary from reflecting unphysical disturbances upstream.

Comparisons with solutions of the linear stability equations[1] show that the method produces highly accurate results. Comparisons with experiments[2] are also presented.

[1] A. Tumin. Receptivity of Pipe Poiseuille Flow. J. Fluid Mech., 315:119–137, 1996

[2] S. Eliahou, A. Tumin, and I. Wygnanski. Laminar–Turbulent Transition in Poiseuille Pipe Flow Subjected to Periodic Perturbation Emanating from the Wall. J. Fluid Mech., to appear

Nonpolynomial spectral method for a singularly perturbed mixed boundary value problem

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In this talk, we discuss an exponentially convergent boundary element approximation of the following mixed boundary value problem:

$$\begin{aligned} \Delta u_\varepsilon &= f \quad \text{in } \Omega \subset \mathbb{R}^2, \\ \partial_n u_\varepsilon &= 0 \quad \text{on } \Gamma_N, \\ \varepsilon \partial_n u_\varepsilon + u_\varepsilon &= g \quad \text{on } \Gamma_R. \end{aligned} \tag{1}$$

Here ε is a small parameter, $\Gamma_N \cup \Gamma_R = \partial\Omega$, and at the points where Γ_N and Γ_R meet, the solution u_ε has singularities whose nature depends on ε. For $\varepsilon > 0$, the singularities are of type $r \log r$ (almost H^2 regularity), whereas for $\varepsilon = 0$, one has the crack-type $\sqrt{r}$ singularities (less than $H^{3/2}$ regularity) of the mixed Dirichlet-Neumann problem.

Similar questions arise in contact problems in elasticity where it was observed numerically that the addition of several singular functions can give very good approximations for small ε.

The precise behavior of u_ε, including a complete asymptotic expansion in powers of ε and corner layer terms, is described in [1]. In this talk, we present estimates in a space of weighted analytic functions with sharp properties of uniformity with respect to the singular perturbation parameter ε.

Then, relying on [2], we consider a boundary integral equation method for the problem (1) and we analyze an "enriched subspace method" for the approximation of u_ε on the boundary $\partial\Omega$. Our method is a p-version BEM augmented by singular functions whose number increases with p. These singular functions are not the singularities of the problem, but their exponents are uniformly distributed in a certain interval. The method gives exponential convergence uniformly in ε.

References

[1] M. Costabel, M. Dauge. A singularly perturbed mixed boundary value problem. *Comm. Partial Differential Equations* **21**, (1996), 1919–1949.

[2] M. Costabel, M. Dauge, M. Suri. Numerical Approximation of a Singularly Perturbed Contact Problem. Prépublication IRMAR 96-29, 1996. To appear in *Computer Methods in Applied Mechanics and Engineering*.

Preconditioning spectral element approximations to the viscous/inviscid coupled problem *

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Abstract The present work follows the subject of [14], and considers preconditionning spectral element approximations to the incompressible viscous/inviscid coupled problem. Before the work of [14], numerical algorithms to solve the resulting discrete coupled equations was always iteration-by-subdomain resolution—known as the alternating Schwarz method. An effective iteration-by-subdomain procedure however requires exact convergence analysis and certain number of repeat resolutions to reach the convergence, which is often theoretically non trivial and numerically expensive. In [14], we introduced a new coupling strategy for viscous/inviscid coupled equations. The new coupling technique allows to solve globally the coupling problem, and hence avoids convergence analysis of the interface iterative procedure and repeat computations. Furthermore, it does not induce additional errors caused by the iteration-by-subdomain procedure, and hence presents more regular transition of the solution between the viscous domain and the inviscid domain at the interface boundaries. This strategy consists in writting the viscous/inviscid coupled equations into a global variational formulation. Thanks to this new weak formulation, the original coupled equations are written under a global saddle problem, similar to the one resulting from the full Stokes equations. Spectral discretizations of such variational formulation take the following form,

$$\begin{pmatrix} \mathbf{H}^- & 0 \\ 0 & \mathbf{H}^+ \end{pmatrix} \begin{pmatrix} \mathbf{u}^- \\ \mathbf{u}^+ \end{pmatrix} - \begin{pmatrix} \mathbf{D}^- & 0 \\ \mathbf{I}^\Gamma & -(\mathbf{D}^+)^T \end{pmatrix}^T \begin{pmatrix} \mathbf{p}^- \\ \mathbf{p}^+ \end{pmatrix} = \begin{pmatrix} \mathbf{B}^-\mathbf{f}^- \\ \mathbf{B}^+\mathbf{f}^+ \end{pmatrix}, \tag{1}$$

$$- \begin{pmatrix} \mathbf{D}^- & 0 \\ \mathbf{I}^\Gamma & -(\mathbf{D}^+)^T \end{pmatrix} \begin{pmatrix} \mathbf{u}^- \\ \mathbf{u}^+ \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{2}$$

where the superscript $-, +$ identify respectively the quantities in the viscous domain and inviscid domain. $\mathbf{u}, \mathbf{p}$ and $\mathbf{f}$ stand for respectively the globally nodal velocity, pressure and augmented force which includes the explicitly treated convective term. $\mathbf{D}$ are the

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discrete gradient/divergence operators. B are the mass matrices. $\mathbf{I}^{\Gamma}$ denotes the discrete interface operator. $\mathbf{H}^k(k = -, +)$ defined by

$$\mathbf{H}^k = \alpha \mathbf{B}^k + \nu \delta_{k-} \mathbf{A}^-$$

where δ_{k-} is the Kronecker symbol, α can be viewed as the inverse of the time step, ν is the viscosity, and $\mathbf{A}^-$ stands for the discrete Laplacien operator.

Therefore standard techniques developped for the Stokes problem can be applied to solve the viscous/inviscid coupled equations. We have chosen the global Uzawa alogorithm to solve the discrete system (1)-(2) for the following raisons: first, between numerous algorithms, the Uzawa decoupling procedure has beeen proven to be attractive in terms of computational complexity and memory requirement than a direct algorithm ([9]); secondly, the bloc diagonal structure in the velocity system allows us to inverse the velocity matrix easily, and therefore reduce the cost in each iteration for the pressure calculation; third, the Uzawa decoupling procedure has been successfully applied to the pure Navier-Stokes solution, choosing the same algorithm to solve the discrete Navier-Stokes/Euler coupled equations enables us to compare the CPU costs with the pure Navier-Stokes solution in an easier way.

Uzawa algorithm decouples the original saddle problem into two positive definite symmetric systems. By this way, the global pressure and global velocity are completely decoupled in the solution process; the pressure **p** is first solved and then the velocity **u** is solved with **p** known. Iterative solution of such systems is feasible and attractive for large problems. In [14] a conjugate gradient iterative algorithm has been applied to solve both the pressure system and the velocity system. However numerical experiments showed that the direct gradient algorithm applied to the pressure algebraic system converges slowly and too many iterations are required to obtain sufficient accuracy.

We present in this work a preconditioning method to accelerate the rate of convergence. We give detailed analysis of the preconditioned Uzawa algorithm, with special emphasis on solving the algebraic equations resulting from spectral element approximation of the Navier-Stokes/Euler coupled equations. Numerical results show that appropriate preconditioner applied to the pressure system can significantly recover the rapid convergence rate, as done by similar preconditioner applied to pure Navier-Stokes pressure system. Thanks to the rapid iterative convergence, the global Uzawa algorithm takes advantages as compared to classical iteration-by-subdomain procedures. Furthermore, generalization of the preconditioned iterative algorithm to flow simulation is carried out. Comparisons of computational complexity between the Navier-Stokes/Euler coupled solution and the full Navier-Stokes solution are made. It is shown that the gain obtained by using the Navier-Stokes/Euler coupled solution is generally considerable.

Keywords Navier-Stokes/Euler coupled equations, spectral element approximation, global Uzawa algorithm, preconditioned conjugate gradient method.

References

[1] Brezzi F., Canuto C., Russo A., *A self-adaptive formulation for the Euler/Navier-Stokes coupling*, Comput. Meth. in Appl. Mech. and Engin., North-Holland, 1989, **73**, p317

[2] Chorin A.J., *Numerical solution of incompressible flow problems*, In J.M. Ortega and W.C. Rheinboldt(ed.), Studies in Numerical Analysis 2, SIAM, 1970

[3] Cahouet J., Chabard J.P., *Some fast 3d finite elements solvers for the generalized Stokes problem*, Int.J.Numer.Meth.in Fluids, 1988, **8**, p869

[4] Debit N., Maday Y., *The coupling of spectral and finite element methods for the approximation of the Stokes problem*, In Proceedings of the 8th France-URSS-Italy joint symposium, Pavie, Italy, 1989

[5] Fischer P., Ronquist E., Dewey D., Patera A.T., *Spectral element methods: Algorithms and Architectures*, In first int. Symp. on domain decomposition methods for partial differential equations, SIAM, 1987, p173

[6] Glowinski R., Pironneau O., *On a mixed finite element approximation of the Stokes problem*, Numer. Math., 1979, **33**, p397

[7] Gastaldi F., Quarteroni A., Sacchi Landriani G., *Effective methods for the treatment of interfaces separating equations of different character*, in Computers and experiments in fluid flow, G.M.Carlomagno and C.A.Brebbia (ed.), Springer-Verlag, Berlin, Heidelberg, New-York, 1989, p65

[8] Kim J., Moin P., *Application of a fractional-step method to incompressible Navier-Stokes equations*, J.Comput.Phys., 1985, **59**, p308

[9] Maday Y., Meiron D., Patera A.T., Ronquist E.M., *Analysis of iterative methods for the steady and unsteady Stokes problem: Application to spectral element discretization*, SIAM J. Sci. Comput. 1993, **14**(2), p310

[10] Maday Y., Patera A.T., *Spectral element methods for the Navier-Stokes equations*, In A.K.Noor (ed.), State-of-the-art surveys in computational machanics, ASME, New York, 1988, p71

[11] Marini L.D., Quarteroni A., *A relaxation procedure for domain decomposition methods using finite elements*, Numer. Math. 1989, **55**, p.575

[12] Orszag S.A., *Spectral methods for problems in complex geometries*, J.Comput.Phys., 1980, **37**, p75

[13] Xu C.J., *A global algorithm on the coupling of Viscous/inviscid equations*, In proceeding of ICOSAHOM'95, Houston J. of Mathematics, 1996, p151

[14] Xu C.J., Maday Y., *Coupling of the Navier-Stokes and Euler equations: Resolution by a spectral method*, In Conference on Scientific and Engineering Computing, National defence industry press, Pekin, 1994

[15] Wathen A., Silvester D., *Fast iterative solution of stabilised Stokes systems*, SIAM J. Numer. Anal., 1993, **30**(3), p630.

Discontinuous Galerkin Spectral/hp Methods on Hybrid Grids

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There has been recently an interesting debate as to what are the relative advantages of structured and unstructured grids, with a renewed interest in cartesian grids for complex-geometry aerodynamic flows [1]. The current confusion stems from the fact that most finite element and finite volume formulations in use today produce solutions which depend strongly on the quality of the grid. Specifically, for highly distorted grids convergence is questionable, and in most cases convergence rates are typically less than second-order. To this end, some - relatively few - efforts have addressed the development of hybrid grids, i.e. a mixture of structured and unstructured grids in order to combine the merits of both discretizations in the context of complex-geometry aerodynamic flows [2], [3], [4]. Such methods lead to more flexible geometric discretization and resolution placement, but they are still of low-order accuracy, i.e. at most second-order.

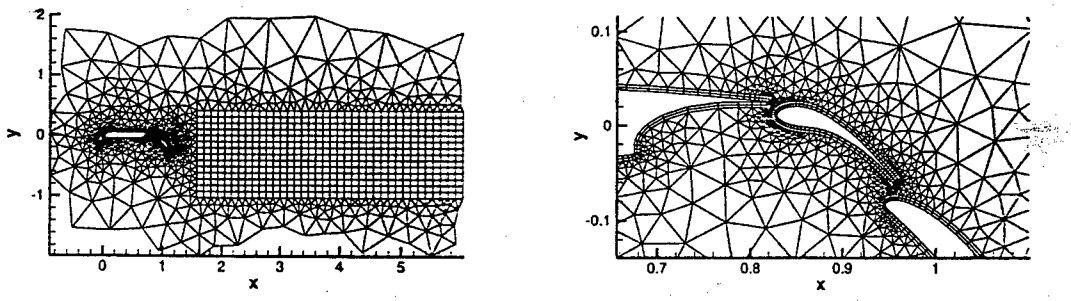

Figure 1: Hybrid discretization around a multi-element airfoil. Only part of the domain is shown.

In the current work we develop a new formulation for 2D and 3D *compressible* Navier-Stokes solutions employing high-order spectral/*hp* element discretization on hybrid grids consisting of triangular and quadrilateral elements in 2D, and of tetrahedra, prisms, hexahedra, and pyramids in 3D. A *discontinuous* Galerkin formulation is developed both for the advection as well as the diffusion contributions that allows multi-domain representation with a discontinuous (i.e. globally L^2) trial basis. This discontinuous basis is orthogonal, hierarchical, and maintains a tensor-product property (even for non-orthogonal elements), a key property for the efficient implementation of high-order methods. Due to this basis orthogonality the resulted mass matrix is diagonal, and thus the proposed method is *matrix-free* given that an explicit time-stepping is involved. The conservativity property is maintained automatically by the discontinuous Galerkin formulation, and monotonicity is controlled by varying the order of the spectral expansion around discontinuities.

An example of a hybrid discretization is shown in figure 1 for simulation of flow past a multi-element airfoil. This problem was studied by Barth [5] who used unstructured disretizations, i.e. only triangles.

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There are two regions of *structured* discretizations as shown in these two plots: First, around the four airfoils where boundary layers are present and where all the vorticity is generated. Second, in the wake region where one single family of square elements is embedded within the unstructured discretization. This uniform meshing minimizes dispersion errors of the traveling vortex street and facilitates maximum storage efficiency.

In the presentation, we will first review the formulation and subsequently present convergence results for an Euler 3D flow, and simulation results of supersonic flow past a NACA4420 airfoil at an angle of attack, of subsonic 2D flow past the multi-element airfoil shown in figures 1, and of 3D flow past a finite span wing.

References

[1] M. Aftosmis, J. Melton, and M. Berger. Adaptation and surface modeling of cartesian mesh methods. In *AIAA-95-1725*, 1995.

[2] V. Parthasarathy, Y. Kallinderis, and K. Nakajima. Hybrid adaption method and directional viscous multigrid with presmatic-tetrahedral meshes. In *AIAA-95-0670, Reno, NV*, 1995.

[3] D.J. Mavriplis and V. Venkatakrishnan. A unified multigrid solver for the Navier-Stokes equations on mixed element meshes. In *AIAA-95-1666, San Diego, CA*, 1995.

[4] D. Tafti, M. Soetrisno, and S. Imlay. A parallel algorithm for hybrid structured-unstructured grids. In *AIAA-96-0287, Reno, NV*, 1996.

[5] T.J. Barth. Steiner triangulization for isotropic and stretched elements. AIAA-95-0213, 1995.

AN OPTIMAL FINITE ELEMENT MULTIGRID PRECONDITIONER FOR CHEBYSHEV-COLLOCATION METHOD

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The spectral-collocation method, being more accurate compared with the finite difference/finite element methods and easier to implement compared with the spectral-tau/spectral-Galerkin methods, has been widely used by scientists and engineers. Since the derivative matrices of the spectral-collocation method are usually full and ill-conditioned, it is now a common practice to precondition them using the derivative matrices of the finite difference/finite element methods with knots at the spectral-collocation points (cf. for instance [4]. [1] and [2]). Although it is generally true and has been proved in many cases that the aforementioned preconditioners are optimal in the sense that the condition numbers of the preconditioned systems are independent of the discretization parameters, however, how to efficiently apply the preconditioner is a great challenge since the grid based on the spectral-collocation points is not quasi-uniform, a condition which is essential to standard finite element and multigrid theory. The aim of this paper is to develop an optimal finite element multigrid preconditioner for the Chebyshev-collocation method.

Consider the following model elliptic problem:

$$\mathcal{L}u := -\nabla \cdot (b\nabla u) = f, \qquad (x,y) \in \Omega = (-1,1)^2, \;\; u|_{\partial\Omega} = 0. \tag{1}$$

We assume that $f(x,y)$ and $b(x,y)$ are sufficiently smooth, and $0 < \alpha \le b(x,y) \le \beta$ for all $(x,y) \in \bar{\Omega}$.

Let $P^0_{N,M}$ be the space of polynomials which are of degree N or less in x and M or less in y and satisfy the homogeneous Dirichlet boundary condition on $\bar{\Omega}$. Then, the Chebyshev-collocation approximation for (1) is to find $u_{NM} \in P^0_{N,M}$ such that

$$(\mathcal{L}u_{NM})(\xi_i,\eta_j) = f(\xi_i,\eta_j), \; 1 \le i \le N-1, \; 1 \le j \le M-1, \tag{2}$$

where the points $\{\xi_i\}_{i=1}^{N-1}$ and $\{\eta_j\}_{j=1}^{M-1}$ are the Chebyshev-Gauss-Lobatto (CGL) points associated with polynomials of degree N and M, respectively.

Let $\bar{u}_{NM}$ and $\bar{f}_{NM}$ be respectively the vectors composed by the values of $u_{NM}(x,y)$ and $f(x,y)$ at $\{\xi_i,\eta_j\}_{1\le i\le N-1,\, 1\le j\le M-1}$, we can rewrite (2) as a linear system

$$L_{sp}\bar{u}_{NM} = W_{NM}\bar{f}_{NM}, \tag{3}$$

where L_{sp} is the Chebyshev spectral differentiation matrix associated to the operator $\mathcal{L}$.

Recently, Kim and Parter [3] proposed an optimal finite element preconditioner for (3) based on the weighted inner product

$$a_\omega(u,v) = \int_\Omega b(x,y)\,\nabla u \nabla v \omega(x,y)\,dxdy,\ \omega(x,y) = (1-x^2)^{-\frac{1}{2}}(1-y^2)^{-\frac{1}{2}}.$$

However, from the implementation point of view, it is preferable in practice to use the standard finite element formulation based on the inner product

$$a(u,v) = \int_\Omega b(x,y)\,\nabla u \nabla v\,dxdy,$$

with which the bilinear finite element approximation to (1) on the CGL grid leads to the linear system

$$L_{fe}\bar{u}_{NM} = M_{fe}\bar{f}_{NM}, \tag{4}$$

where L_{fe} and M_{fe} are respectively the stiffness and mass matrices associated with bilinear finite elements with knots at the CGL points.

Although it appears unnatural to precondition the Chebyshev-collocation system (3) without using the (Chebyshev) weighted inner product, we will show that ${M_{fe}}^{-1}A_{fe}$ is indeed an optimal preconditioner for L_{sp}, i.e. (4) provides an optimal preconditioner for (3).

The linear system (4) is derived from a bilinear finite element approximation on the CGL grid which is not quasi-uniform. Hence, standard multigrid techniques applied to (4) converge very slowly. We will present a new optimal multigrid preconditioner for (4) by taking into account the special structure of the CGL grid. Hence, by using a suitable generalized conjugate gradient method, the overall computational complexity of solving (3) is quasi-optimal (optimal up to a logarithmic term) thanks to the fast Fourier transform and the new optimal multigrid preconditioner. We will also present extensive numerical results which indicate that this algorithm is not only very efficient but also robust in the sense that the convergence rate is insensitive to the ratio $\frac{\max_\Omega b(x,y)}{\min_\Omega b(x,y)}$.

REFERENCES

[1] C. Canuto and A. Quarteroni. Preconditioner minimal residual methods for Chebyshev spectral calculations. *J. Comput. Phys.*, 60:315–337. 1985.

[2] M. O. Deville and E. H. Mund. Chebyshev pseudospectral solution of second-order elliptic equations with finite element preconditioning. *J. Comput. Phys.*, 60:517–533, 1985.

[3] S. D. Kim and S. V. Parter. Preconditioning chebyshev spectral collocation method for elliptic partial differential equations. *SIAM J. Numer. Anal.*, 33, No. 6:2375–2400, 1996.

[4] S. A. Orszag. Spectral methods for complex geometries. *J. Comput. Phys.*, 37:70–92, 1980.

Spectral influence matrix without corner pathology

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The use of the influence matrix is very common in the solution of the incompressible Navier–Stokes equations by means of spectral methods. This technique is however faced with a difficulty when applied to problems with two or three nonperiodic spatial directions. In fact, the influence matrices evaluated for *tau* and collocation Chebyshev spectral approximations to the u-p [4] and ω-ψ [3] equations have been found to possess a number of singularities related to the number of corners of the computational domain.

This kind of difficulty seems strictly related to the spatial discretizations by spectral methods since it has not been observed when the same uncoupled methods are applied to the equations discretized spatially by finite differences or finite elements, *cf.* [5]. The singular nature of the spectral influence matrices implies that they cannot be inverted unless a special treatment is adopted to eliminate the spurious modes associated with the space of the zero eigenvalue. Effective *ad hoc* procedures have been proposed in the aformentioned works and are analyzed in [11] and [6]. In a Chebyshev-*tau* method for solving the ω-u Navier–Stokes equations, the singularity of the influence matrix for the determination of the boundary value of vorticity has been avoided by a not entirely justified amputation of the corner values of this variable [2].

Recently, the development of spectral methods has witnessed a trend toward the use of the Galerkin method to exploit the well know advantages stemming from the variational formulation of boundary value problems for elliptic operators, see, *e.g.*, [1] and [9]. In particular, fast elliptic Poisson spectral solvers using diagonalization techniques within the context of the

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standard Galerkin method have been proposed using Legendre or Chebyshev polynomials [10]. Therefore, these new spectral solution algorithms should allow to reanalyze the issue of the singular nature of spectral influence matrices for the calculation of incompressible viscous flows in 2D and 3D, to find eventually a conceptually more satisfactory solution than the ones proposed so far.

The aim of this paper is to describe a Galerkin–Legendre method for the uncoupled solution of the vorticity and stream function equations in which the influence matrix for the determination of the vorticity boundary value is free from any singular behaviour. The method is based on implementing conditions of an integral kind for the vorticity [7] in the format of the Glowinski–Pironneau method, conveniently expressed according to the considerd spectral approximation. This means that one can get rid of the explicit construction of the harmonic functions occurring in the vorticity integral conditions but has to evaluate volume integrals involving the surrogate functions with same trace as the harmonic functions. At variance with the original finite-element method of Glowinski and Pironneau, the integration extends here over the entire domain instead of being limited to the shell of elements in contact with the boundary. However, by virtue of the high sparsity of matrices associated with the Legendre polynomials combined with the direct product nature of the 2D spectral approximation, the full-volume integrals can be evaluated fast enough to build an efficient solver for the biharmonic problem expressed as a system of two second-order elliptic equations.

Let us consider the Navier–Stokes equations for 2D flows expressed in terms of the variables vorticity ζ and stream function ψ. Taking into account the nonlinear advection term explicitly, the equations discretized in time can be written in the following uncoupled form [7]

$$\begin{aligned} (-\nabla^2 + \gamma)\zeta &= f, \qquad \int_\Omega \zeta\eta = \oint_{\partial\Omega} \left(a\frac{\partial\eta}{\partial n} - b\eta \right), \\ -\nabla^2\psi &= \zeta, \qquad \psi_{|\partial\Omega} = a, \end{aligned}$$

where $\gamma = \mathrm{Re}/\Delta t$, $f = \gamma\zeta^{\mathrm{old}} - \mathrm{Re}J(\zeta^{\mathrm{old}}, \psi^{\mathrm{old}})$, and $\zeta = \zeta^{\mathrm{new}}$ and $\psi = \psi^{\mathrm{new}}$. In the integral conditions above, η represents any function harmonic in the computational domain Ω, and (a, b) denote the boundary data for ψ and $(\partial\psi/\partial n)$, respectively, which can be expressed in terms of the velocity specified on the boundary $\partial\Omega$. Note that the Dirichlet datum a is assumed to be continuous at the four corners, see, for instance, [1, p. 93], whilst the Neumann datum b is not required to satisfy such a condition.

The spatial discretization of the ζ-ψ equations is done by means of the Galerkin spectral method based on the Legendre polynomials $L_n(x)$, $n \geq 0$. Let us consider the basis for representing functions of $x \in [-1, 1]$:

$$\{L_n^*(x),\ 0 \leq n \leq N\} \equiv \{1,\ x/\sqrt{2},\ k_{n-1}(1-x^2)L'_{n-1}(x),\ 2 \leq n \leq N\},$$

where $k_n \equiv (\sqrt{n+1/2})/(n+n^2)$. Thus $L_n^*(x)$ is a polynomial of degree n for any $n \geq 0$ and for $n \geq 2$ one has Shen's basis [10]

$$L_n^*(x) = \frac{L_{n-2}(x) - L_n(x)}{\sqrt{2(2n-1)}}.$$

The normalization of $L_n^*(x)$ has been chosen to make the stiffness matrix coincident with the unit matrix of proper dimension (but for the constant mode). The approximate solution ζ_N is expanded in the double series

$$\zeta_N(x,y) = \sum_{i=0}^{I}\sum_{j=0}^{J} L_i^*(x)\,\zeta_{i,j}\,L_j^*(y),$$

and similarly for ψ_N.

To enforce the vorticity integral conditions according to the Glowinski–Pironneau method, one has to introduce auxilliary functions w to replace the basis of the harmonic functions η. We define the basis $\{w^k(x,y),\ 1 \leq k \leq 2(I+J)\}$ as follows

$$\begin{cases} w^i(x,y) = L_i^*(x), & w^{I+1+i}(x,y) = L_i^*(x)\frac{y}{\sqrt{2}}, & 0 \leq i \leq I, \\ w^{2I+1+j}(x,y) = L_j^*(y), & w^{2I+J+j}(x,y) = \frac{x}{\sqrt{2}}L_j^*(y), & 2 \leq j \leq J. \end{cases}$$

As a consequence of this representation, the component $\zeta_N^{(\mathrm{int})}$ of the vorticity field which accounts for the fulfillment of the integral conditions will be expressed as follows:

$$\zeta_N^{(\mathrm{int})}(x,y) = \sum_{i=0,1}\sum_{j=0,1} L_i^*(x)\,\zeta_{i,j}\,L_j^*(y) + \sum_{i=2}^{I} L_i^*(x)\Big[\zeta_{i,0} + \zeta_{i,1}\frac{y}{\sqrt{2}}\Big] + \sum_{j=2}^{J}\Big[\zeta_{0,j} + \frac{x}{\sqrt{2}}\,\zeta_{1,j}\Big]L_j^*(y).$$

The influence matrix of order $2(I+J)$ is constructed using this basis and is found to be nonsingular, as it should be. A detailed description of the matrix operations used to evaluate its coefficients will be given in the final paper.

We have first applied the uncoupled algorithm to the solution of the biharmonic problem (Re = 0), assuming the boundary conditions of the driven cavity problem, *without* any regularization: namely, the Neumann datum is kept discontinuous at the two upper corners. Although the solution of such a biharmonic problem is singular there, the present direct method provides a correct discrete solution which satisfies the global conservation law $\int_\Omega \zeta_N = -\oint_{\partial\Omega} b$—exactly, within round-off errors. The latter is in fact nothing but the integral condition with respect to the harmonic function $\eta(x,y) \equiv 1$.

Then, we have considered the nonlinear problem for Re = 1000 using $\Delta t = 0.025$ and $I = J = 100$. The plots of ζ and ψ at $t = 100$ are shown in the figures which demonstrate that the ω-ψ spectral solutions can be computed without the need of regularizing the velocity boundary data.

In the present calcuations we purposely did not subtract the singular component of the (steady) solution to demonstrate that a spectral solution can be computed irrespective of the high singular behaviour of the vorticity field. The presence of spatial oscillations in ζ at the smallest wavelenghts is however an indication that an appropriate treatment of the solution singularity will improve the accuracy of its spectral counterpart.

It can be remarked that the proposed method provides also some guidelines to develop Legendre spectral schemes for the uncoupled solution of the primitive variable Navier–Stokes equations. In fact, provided that the influence operator for determining the trace of pressure is characterized by the pressure integral conditions introduced in [8], a spectral influence matrix will be obtained not plagued by pathological singularities,

References

[1] C. Bernardi and Y. Maday, *Approximations spectrales des problèmes aux limites elliptiques*, Springer-Verlag, Paris, 1992.

[2] H. J. H. Clercx, A spectral solver for the Navier–Stokes equations in the velocity–vorticity formulation for flows with two nonperiodic directions, *J. Comput. Phys.*, **137** (1997) 186–211.

[3] U. Ehrenstein and R. Peyret, A Chebyshev collocation method for the Navier–Stokes equations with application to double-diffusive convection, *I. J. Numer. Meth. Fluids*, **9** (1989) 427–452.

[4] P. Le Quéré and T. Alziary de Roquefort, Computation of natural convection in two-dimensional cavities with Chebyshev polynomials, *J. Comput. Phys.*, **50** (1985) 210–228.

[5] M. Napolitano, G. Pascazio and L. Quartapelle, A review of vorticity conditions for the solution of the ζ-ψ equations, *Computers and Fluids*, to appear, 1998.

[6] R. Peyret, Spectral methods for the vorticity–streamfunction equations, *Computational Fluid Dynamics Review*, Eds. M. Hafez and K. Oshima, John Wiley and Sons, 1997.

[7] L. Quartapelle, *Numerical Solution of the Incompressible Navier–Stokes Equations*, Birkhäuser, Basel, 1993.

[8] L. Quartapelle and M. Napolitano, Integral conditions for the pressure in the computation of incompressible viscous flows, *J. Comput. Phys.*, **60** (1986) 340–348.

[9] A. Quarteroni and A. Valli, *Numerical Approximation of Partial Differential Equations*, Second Printing, Springer-Verlag, Berlin, 1997.

[10] J. Shen, Efficient spectral–Galerkin method I. Direct solvers for second- and fourth-order equations using Legendre polynomials, *SIAM J. Sci. Comput.*, **15** (1994) 1489–1505.

[11] L. Tuckerman, Divergence-free velocity fields in nonperiodic geometries, *J. Comput. Phys.*, **80** (1989) 403–441.

A Finite Element Preconditioner for Non-Linear Stokes Equations using a Spectral Element Method

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The development of efficient tools for the numerical simulation of three-dimensional fluid-flow problems has received much attention over the last decade. Numerous theoretical and algorithmical developments opened the possibilities of spectral methods to solve complex flow problems. For these large-scale simulations iterative methods are necessary and several techniques were proposed [1, 2]. In this work a numerical scheme and iterative solver are presented to solve the unsteady Navier–Stokes equations for a generalized Newtonian fluid in a complex geometry. The diffusion coefficient becomes non-linear and hence each time step a new system of equations has to be solved. The equations are integrated in time using a splitting procedure and then discretized spatially by means of a high order spectral element method. We propose a numerical solution strategy where a static finite element preconditioner is used to limit the number of required iteration steps. Some results are given where the clustering of the eigenvalues is analyzed. Finally results are presented for the fluid flow in a static mixer, a complex three dimensional geometry.

In order to model a general viscous fluid one needs to solve the system

$$\begin{cases} \dfrac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} = -\nabla p + \nabla\cdot 2\eta(\dot{\gamma})\,\mathbf{D} + \mathbf{f} \\ \nabla\cdot\mathbf{v} = 0, \end{cases}$$

where η is the variable viscosity and $\dot{\gamma}$ the shear-rate defined as $\dot{\gamma} = \sqrt{2\mathrm{tr}(\mathbf{D})^2}$ and $\mathbf{D} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^c$ the rate of deformation tensor. The non-linearity in convection and diffusion calls for an efficient numerical technique. A scheme for the above equations is proposed, based on an operator-integration-factor splitting [3, 4] for the non-linear convection term and a projection scheme to decouple the pressure and velocity.

For the spatial discretization a high-order Galerkin spectral element method is chosen, that exhibits excellent properties with respect to numerical diffusion and dispersion. For stability reasons it is shown that an implicit treatment of the non-linear diffusion is preferably. This requires the assembly and solution of a system of equations of the form $-\nabla\cdot 2\eta(\dot{\gamma})\,\mathbf{D} + \lambda\,\mathbf{u} = \mathbf{h}$

each time step. Here we present a conjugate gradient based iterative solver with a static finite element preconditioner $\mathbf{F}$ to solve the discretized system $\mathbf{Su} = \mathbf{h}$. Only residual vectors are required each time step, which can be computed on elemental level, significantly lowering the memory requirements.

The clustering of the eigenvalues of the matrix $\mathbf{F}^{-1}\mathbf{S}$ is investigated for both increasing polynomial order and number of elements. For a model 2D-case the eigenvalue distribution is presented in Fgure ??, showing a reduction of the condition of more than $\mathcal{V}(10^5)$. The time to solve a non-linear problem is approximately a factor 2.5 higher than for the constant viscosity problem. The memory requirements are approximately the same. An application of the algorithm is presented for a non-Newtonian fluid flow in a complex geometry. The velocity field in flow direction is here presented in Figure ??.

References

[1] P.F. Fisher Parallel multi-level solvers for spectral element methods *Proceedings of ICOSAHOM 1995, Houston, Texas.*

[2] W.Couzy Iterative solutions of the 3D transient Navier–Stokes equations on parallel computers *Proceedings of ICOSAHOM 1995, Houston, Texas.*

[3] Y. Maday, A. T. Patera, and E. M. Rønquist. An operator-integration-factor splitting method for time-dependent problems: application to incompressible fluid flow. *Journal of Scientific Computing*, 5:263–292, 1990.

[4] L. J. P. Timmermans, P. D. Minev, and F. N. van de Vosse. An approximate projection scheme for incompressible flow using spectral elements. *International Journal of Numerical Methods in Fluids*, 1996.

ICO98-63

Iterative Substructuring Methods for Spectral Elements Discretizations of Saddle Point Problems

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We introduce and discuss some nonoverlapping domain decomposition preconditioners for the efficient iterative solution of saddle point problems with a penalty term discretized with mixed spectral element methods. Examples of such problems are Stokes and linearized Navier-Stokes equations and mixed formulations of linear elasticity. These problems have the discrete form:

$$\begin{bmatrix} A & B^T \\ B & -t^2 C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix}, \tag{1}$$

where the penalty term $-t^2 C$ depends on the Poisson ratio for elasticity problems or on stabilization parameters for flow problems.

Several iterative methods have been proposed and studied in the case of low-order h-version finite elements, such as Uzawa's algorithm, multigrid, preconditioned conjugate gradient and preconditioned conjugate residuals. Here we consider instead spectral and p-version finite elements, in particular the $Q_n - Q_{n-2}$ and $Q_n - P_{n-1}$ methods. Already for scalar problems, the stiffness matrices obtained by spectral discretizations are less sparse and more ill-conditioned than those obtained with h-version finite elements. For saddle point systems, there is the additional problem of the nonuniform stability (in the sense of the inf-sup condition) of many spectral discretizations.

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The construction and analysis of efficient and scalable iterative methods is therefore more challenging.

Using a substructuring technique well-known for positive definite problems, we implicitly eliminate all the variables (velocities and pressures) associated with the interior of each spectral element. The resulting saddle point Schur complement, involving the interface velocities $\mathbf{u}_\Gamma$ and the coarse pressures p_0 that are constant in each element, has the form

$$\begin{bmatrix} S_\Gamma & B_0^T \\ B_0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_\Gamma \\ p_0 \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{b}} \\ 0 \end{bmatrix}. \tag{2}$$

We solve this reduced saddle point problem with a Krylov space method with a block-diagonal or block-triangular preconditioner

$$\widehat{D} = \begin{bmatrix} \widehat{S}_\Gamma & 0 \\ 0 & \widehat{C}_0 \end{bmatrix} \qquad \widehat{T} = \begin{bmatrix} \widehat{S}_\Gamma & 0 \\ B_0 & -\widehat{C}_0 \end{bmatrix},$$

where $\widehat{S}_\Gamma$ and $\widehat{C}_0$ are good preconditioners for S_Γ and the coarse pressure mass matrix C_0, respectively. For the velocity block, we use substructuring preconditioners of wire basket type. For example, each interface velocity component in the Stokes case can be preconditioned with the scalar wire basket preconditioner studied in [4]:

$$\widehat{S}_W^{-1} = R_0 \widehat{S}_{WW}^{-1} R_0^T + \sum_k R_{F_k} \widehat{S}_{F_k F_k}^{-1} R_{F_k}^T.$$

This is an additive preconditioner with independent solvers $\widehat{S}_{F_k F_k}^{-1}$ for each face F_k and a coarse solver $\widehat{S}_{WW}^{-1}$ for the wire basket W of the elements. Other substructuring preconditioners, such as the Neumann-Neumann preconditioner, could also be used and these techniques can be extended to elasticity problems. For the resulting algorithms, we prove that the condition number of the preconditioned operator is bounded by

$$C \frac{(1 + \log n)^2}{\beta_n},$$

where C is independent of n and N, and β_n is the discrete inf-sup constant of the mixed spectral discretization employed.

This is joint work with O.B. Widlund of the Courant Institute of Mathematical Sciences, New York University, USA.

References

[1] C. BERNARDI AND Y. MADAY, *Approximations Spectrales de Problèmes aux Limites Elliptiques*, vol. 10 of Mathèmatiques & Applications, Springer-Verlag France, Paris, 1992.

[2] F. BREZZI AND M. FORTIN, *Mixed and Hybrid Finite Element Methods*, Springer-Verlag, 1991.

[3] C. CANUTO, M. Y. HUSSAINI, A. QUARTERONI, AND T. A. ZANG, *Spectral Methods in Fluid Dynamics*, Springer-Verlag, Berlin, 1988.

[4] L. F. PAVARINO AND O. B. WIDLUND, *A polylogarithmic bound for an iterative substructuring method for spectral elements in three dimensions*, SIAM J. Numer. Anal., 33 (1996), pp. 1303–1335.

[5] L. F. PAVARINO, *Preconditioned conjugate residual methods for mixed spectral discretizations of elasticity and Stokes problems*, Comp. Meth. Appl. Mech. Engr., 146 (1997), pp. 19–30.

[6] L. F. PAVARINO AND O. B. WIDLUND, *Iterative substructuring methods for spectral element discretizations of elliptic systems. II: mixed methods for linear elasticity and Stokes flow*, Tech. Rep. 755 , Dept. of Computer Science, Courant Institute of Mathematical Sciences, 1997.

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ICOSAHOM 98

Abstract

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Adaptive mapping for the p−version of the finite element method using NURBS

In order to provide an exact mapping for complex geometries the blending function method must be used. For applying the blending function method the bounding edges $x_i(\lambda), i = 1,2,3,(4)$ of the finite elements have to be parameterized with respect to a parameter λ. For the parametric description of the edges the following methods can be used:

- exact representation (explicit parametric curve)
- approximation by interpolation polynomials
  - using uniform interpolation
  - using special collocation point sets (Chebishev points, L^∞ minimal interpolation point sets etc.)
- approximation by $B-$splines or non-rational $B-$splines.

The explicit parameterization of the curves [3] is the preferred method when applicable. However, for some cases either the exact parametric representation is not available (intersection curves), or for some reason, it is not applicable (e.g. the parameterization is not uniform). The use of interpolation polynomials [2] is a viable alternative but the increase of the accuracy of the approximation requires that the degree of the interpolating polynomials be increased. However, for some functions the increase of the degree of the interpolating polynomial will increase the error of the approximation. Using non-uniform interpolation point sets will provide a better approximation (by significantly decreasing the

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Lebesque constant of the interpolation operator) [1], although there is no interpolation point set that will guarantee the convergence when approximating an arbitrary continuous function. Another problem is the continuity of the function values and the continuity of the derivatives (or having a prescribed value) between elements. Generally the usage of special interpolation point sets (for example the L^∞ minimal interpolation point sets) will produce a better result in that respect. The numerical evaluation of higher order interpolation polynomials is unstable (especially when using a Vandermonde type matrix for calculating the interpolation polynomials, since the condition numbers of these matrices are very large).

In this paper the use $B-$splines or non-rational $B-$splines (NURBS) for the parametric description of the edges is discussed. NURBS provide a possibility for exact boundary representation for a wide class of functions (for example conic sections). The usage of cubic splines will also guarantee enough flexibility for approximating any continuous functions at any degree of accuracy. By increasing the number of interpolation points the interpolating $B-$spline curve will converge to the approximated boundary curve for any continuous curve. Also, using canonical interpolation, the continuity of the boundary curves between elements is guaranteed. By specifying the first and second derivatives (for cubic splines) between elements will guarantee the continuity of these derivatives or will provide the required value of the derivatives (at corners for example). The evaluation of splines is stable. The round-off error of the evaluation of splines does not depend on the number of interpolation points. Another advantage is that the speed of the evaluation of the spline curves is considerably faster than the evaluation of higher order polynomials.

Examples are presented.

References

[1] Qi Chen and Ivo Babuška. Approximate optimal points for polynomial interpolation of real functions in an interval and in a triangle. *Comput. Methods Appl. Mech. Engrg*, 128:405–417, 1995.

[2] György Királyfalvi and Barna A. Szabó. Quasi-regional mapping for the p-version of the finite element method. *Finite Elements in Analysis and Design*, 27:85–97, 1997. Special Issue: Robert J. Melosh Medal Competition.

[3] Barna A. Szabó and Ivo Babuška. *Finite element analysis.* John Wiley & Sons, Inc., New York, 1991.

hp–FEM for the Stokes problem

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Abstract

The efficient and accurate numerical solution of fluid mechanics problems is nowadays of significant engineering interest and the aim of this paper. These problems are often difficult to solve accurately due to the presence of corner singularities and boundary layers. Although the solutions of fluid flow problems exhibit these phenomena, they are typically piecewise analytic. In this case it is well known that the use of the *hp* version of the Finite Element Method (FEM) can lead to exponential rates of convergence. For a corner singularity this exponential convergence rate is obtained by increasing the polynomial approximation order and refining the mesh geometrically towards the singularity. This local mesh refinement, using possibly irregular meshes with hanging nodes and non constant polynomial degree, is implemented in our code HP90, compare [1].

Stability of the classical mixed Galerkin FEM discretization for viscous incompressible fluid flow is guaranteed as long as the discrete inf-sup or Babuška-Brezzi condition is satisfied by the velocity and the pressure spaces. This condition has been established for various velocity and pressure space pairings for the *h*-, *p*-, *hp*-version as well as the spectral FEM.

Implementationally very attractive pairings, such as equal-order elements for the velocity and the pressure, do not fulfill this stability condition and lead to unphysical spurious pressure modes in computations. Stabilized mixed methods, compare [2] and the references therein, avoiding this stability problem have emerged. Regarding the *h* version FEM such stabilized methods have already been applied to a variety of problems in fluid flow, elasticity and continuum mechanics. An *hp* Galerkin Least Squares (GLS) approach based on equal order spaces is analyzed in [3,4] for the Stokes problem and exponential rates of convergence are established.

The comparison of the mixed Galerkin and the GLS formulation for the Stokes problem in the context of the above *hp* FEM is the goal of this paper. We present these two formulations and their implementation in HP90, which is a general *hp* FE code. For a backward facing step flow problem with a singular solution, we

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obtain for both methods exponential rates of convergence. We discuss the practical (implementational) advantages and disadvantages of both methods.

We show theoretical results for both formulations and confirm them by a numerical convergence study. Our numerical experiments clearly indicate the exponential convergence for the Galerkin and GLS *hp*–FEM, as predicted by the theory.

References

[1] L. Demkowicz, K. Gerdes, C. Schwab, A. Bajer and T. Walsh. HP90: A general & flexible Fortran 90 *hp*-FE code. SAM Report 97-17, submitted to Computing and Visualization in Science.

[2] L.P. Franca, T.J.R. Hughes and R. Stenberg. Stabilized Finite Element Methods. *Incompressible Computational Fluid Dynamics: Trends and Advances*, editors M.D. Gunzburger and R.A. Nicolaides, Cambridge University Press, 1993.

[3] K. Gerdes and D. Schötzau. *hp* FEM for incompressible fluid flow – stable and stabilized. SAM Report 97-18, submitted to International Journal for Numerical Methods in Engineering.

[4] D. Schötzau, K. Gerdes and C. Schwab. Galerkin Least Squares *hp*-FEM for the Stokes problem. In press in *Comptes Rendus de l'Académie des Sciences Paris.*

Fast Solvers for Boundary Integral Equations for Electric Screens.

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We consider time-harmonic Maxwell's equations in the exterior Ω of an open, perfectly conducting surface Γ where the tangential component of the electric field on Γ is given:

$$\begin{gathered}\operatorname{curl}\mathbf{E}=\mathbf{H},\quad \operatorname{curl}\mathbf{H}=k^2\mathbf{E}\quad \text{in } \Omega,\\ n\times\mathbf{E}=\mathbf{g}\quad \text{on } \Gamma,\\ \mathbf{H}\times\tfrac{x}{|x|}-\mathbf{E}=o(\tfrac{1}{|x|})\quad \text{for } |x|\to\infty.\end{gathered}$$

Here, $g=-n\times\mathbf{E}^0$ for a given incident electric field $\mathbf{E}^0$ and $\mathbf{E}$ and $\mathbf{H}$ denote the scattered electro-magnetic field, and n is the normal vector to the screen Γ. The wave number k is assumed to be real and not too large. A well-known ansatz for the solution is $\mathbf{E}=V_k(\mathbf{J})+\operatorname{grad}V_k(M)$, $\mathbf{H}=\operatorname{curl}V_k(\mathbf{J})$ for unknown fields $\mathbf{J}$ and M with the single layer potential

$$V_k(M)(x):=\frac{1}{4\pi}\int_\Gamma M(y)\frac{e^{ik|x-y|}}{|x-y|}\,dS_y\quad (x\in\Gamma).$$

This ansatz leads to the strongly elliptic system of integral equations

$$\begin{aligned}n\times V_k(\mathbf{J})+n\times\operatorname{grad}_\Gamma V_k(M) &= \mathbf{g},\\ \operatorname{div}\left(n(n\cdot V_k(\mathbf{J}))\right)-(\Delta_\Gamma+k^2)V_k(M) &= \operatorname{div}_\Gamma n\times\mathbf{g},\end{aligned}$$

which is in general non-Hermitian and indefinite. Its solution inherits possible corner and corner-edge singularities of the electro-magnetic fields. We consider the p-version of the Galerkin method to solve the system of integral equations, which converges at least twice as fast as the h-version. On the other hand, since we deal with first kind integral equations, the linear systems of the Galerkin method are ill-conditioned, which becomes even worse for high polynomial degrees of the ansatz functions. We also note that in general the systems are fully occupied since the integral operators couple also functions with disjoint supports.

We present preconditioners which substantially reduce the numbers of iterations of the generalized conjugate residual method (GMRES) for the solutions of the linear systems. Our preconditioners are of the additive Schwarz type which require the solutions of a couple of local problems and of a low dimensional global problem. The individual problems again are discrete forms of boundary integral equations.

The ansatz space for the Galerkin method has three components, $X = X_1 \times X_2 \times X_3$, two for the tangential field $\mathbf{J}$ and one for the scalar field M. The components X_1 and X_2 are subspaces of the energy space of the single layer potential which is weakly singular. Therefore, X_1 and X_2 may contain discontinuous functions. On the other hand the component X_3 is a subspace of the energy space of the operator $-(\Delta_\Gamma + k^2)V_k$, which is hyper-singular. Thus, for X_3 we need to consider continuous functions. In our model problem we deal with rectangular meshes on rectangular screens. For X_1 and X_2 we take on each of the elements tensor-products of Legendre polynomials which may be globally discontinuous. For X_3 we take tensor-products of anti-derivatives of Legendre polynomials to ensure global continuity.

To define preconditioners we consider (besides a small global problem) decompositions of the spaces X_1, X_2 and of X_3, separately. Here we also need to consider coarse spaces for low-dimensional global problems within the components, and a couple of local subspaces. The local projections can be defined with respect to the original indefinite integral operators as well as with respect to their main, positive definite parts.

The decompositions of the components X_1 and X_2 can be non-overlapping since continuity is not required. Here, an essential point is that functions of the local subspaces must have integral-mean zero. Decompositions of the component X_3 have to take continuity into consideration. This can be dealt with by overlapping decompositions, which lead to fast iterative methods with respect to the required number of iterations. In this case, due to the overlaps, the individual local problems are relatively large and are therefore rather expensive to be solved. It turns out that the use of discretely harmonic basis functions allows for further decomposing the individual local subspaces of X_3. Even the diagonal scaling is sufficient when taking these basis functions.

By canonically assembling the preconditioners for the three components X_1, X_2, and X_3 we end up with preconditioners for the whole Galerkin system of boundary integral equations. The efficiency of the methods is demonstrated by numerical experiments.

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An h-p adaptive spectral element method for the Stokes problem

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Spectral element methods exhibit exponential rates of convergence when the solution to the problem being solved is infinitely smooth. However, the successful and cost-effective implementation of such methods for problems where the domain is not smooth or the solution to the problem has a boundary layer, depends on a suitable decomposition of the domain into spectral elements and an appropriate choice for the order of polynomial representation within each element. The two important issues in an adaptive method are a suitable 'a posteriori' error estimate based on the approximation to the solution and the decision on whether an h-refinement or p-enrichment should take place in an element where a prescribed level of accuracy has not been achieved.

In this paper we use a non-conforming h-p adaptive spectral element method to solve swirling Stokes flow in a rotating cylinder. The method allows an arbitrary number of non-overlapping elements within the domain, flexibility in the configuration of elements and any polynomial order of approximation in each spatial direction. This method has advantages over a conforming spectral element method as the preservation of C^0-continuity in the latter leads to refinements and/or enrichments in the polynomial order of approximation in elements where the prescribed level of accuracy has already been achieved, thereby using more degrees of freedom than is necessary. Minimisation of the jump of the solution between adjacent elements is imposed using the mortar element method (see [1]) extended to the case of different polynomial orders of approximation amongst the elements in the mesh.

The h-p adaptive strategy described in this paper features an element residual 'a posteriori' error estimate (see [4]), equidistribution of the global error amongst the elements in the mesh and simultaneous h and p refinements. In [2], this strategy was proved to outperform the three step strategy developed by Oden *et al* [3] for a one-dimensional boundary value problem.

We distinguish two stages in the algorithm and use the superscripts 'old' and 'new' to denote the current and next iterations respectively and the index i to denote the ith-element. First the initial mesh details are specified and afterwards the h and p refinements are carried out. For a one-dimensional problem the strategy then proceeds as follows:

(i) **Initial mesh details.** The adaptive scheme starts by defining a global target error θ^{tgt} as well as an initial number of elements s^{old} and lengths and polynomial approximation orders for each element, h_i^{old}, p_i^{old}. Then, a numerical solution takes

place to give local and global error indicators θ_i^{old} and θ^{old}. Then, an elemental target error $(\theta^{tgt})_i^{old}$ is obtained for each element based on equidistribution of the initial target global error over the initial mesh, i.e. $(\theta^{tgt})_i^{old} = \frac{\theta^{tgt}}{\sqrt{s^{old}}}$.

(ii) h **and** p **refinements.** h-refinements or p-enrichments will take place until the global target error θ^{tgt} is met. We start this process by estimating the local regularities m_i for each element. If the local error target $(\theta^{tgt})_i^{old}$ has not been achieved and the local regularity within an element $m_i \leq p_i^{old} + 1$, the element is refined and the new elemental target error $(\theta^{tgt})_i^{new}$ is found by equidistributing the original elemental target error among its 'sons':

$$(\theta^{tgt})_i^{new} = \frac{(\theta^{tgt})_i^{old}}{\sqrt{\tilde{n}}}$$

where $\tilde{n}$ is the number of subdivisions. No p-enrichment takes place. If the local error target $(\theta^{tgt})_i^{old}$ has not been achieved and the local regularity $m_i > p_i^{old} + 1$ then the order of the polynomial approximation p_i^{new} is taken as $p_i^{old} + 1$. Now, the number of elements s^{new}, order of polynomial approximations p_i^{new}, lengths of the elements h_i^{new} and elemental target errors $(\theta^{tgt})_i^{new}$ are updated, a new numerical solution is carried out and the new global error θ^{new} is recalculated. If this new global error θ^{new} is less than or equal to the global error target θ^{tgt} the process finishes, otherwise the h and p refinements continue.

Results of a computation on a non-conforming mesh for swirling Stokes flow where the exact solution is known are shown below.

Several examples of how this strategy successfully guides the non-conforming mortar element approximation while achieving a good compromise between accuracy and computational cost measured in terms of global number of degrees of freedom and cpu-time will be presented at the conference.

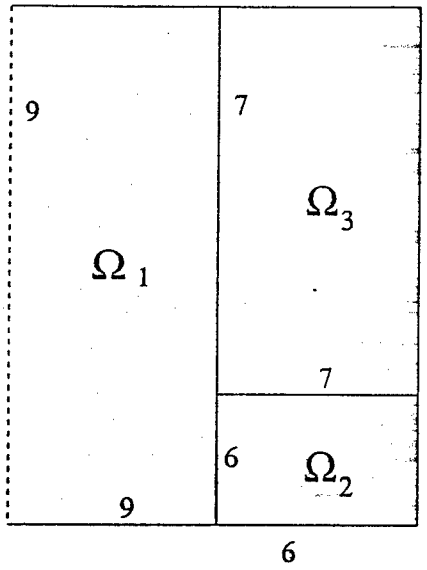

Figure 0.1: Mesh and polynomial orders

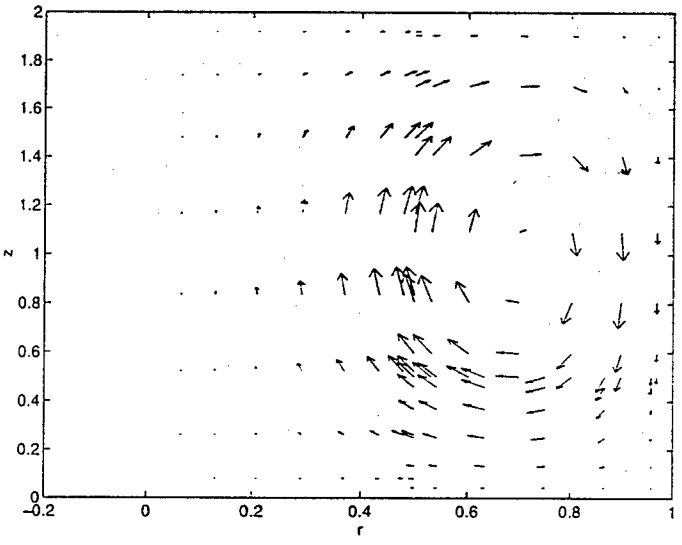

Figure 0.2: Approximated velocity field for test1

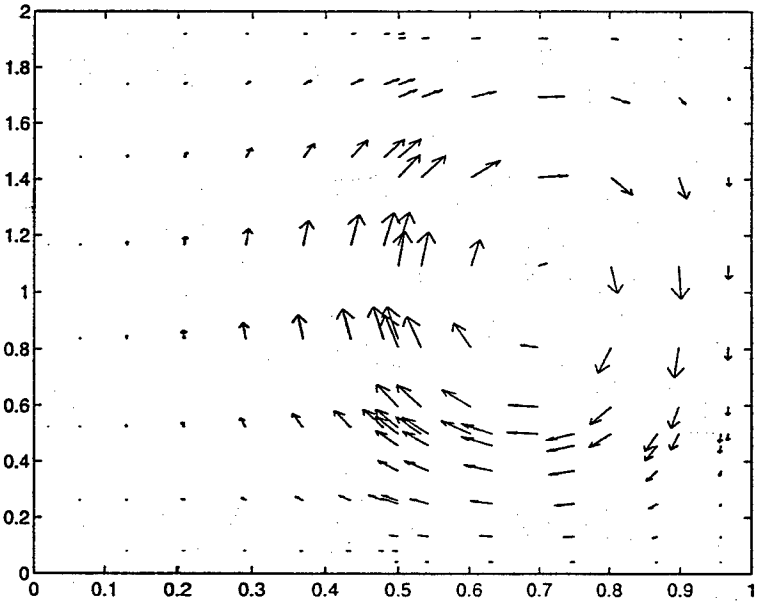

Figure 0.3: Exact velocity field

Bibliography

[1] C. Bernardi, Y. Maday, and A.T. Patera. A new nonconforming approach to domain decomposition: the mortar element method. In H. Brezis and J.L. Lions, editors, *Nonlinear partial differential equations and their applications, Collège de France Seminar*, volume XI of *Pitman Research Notes in Mathematics Series*, pages 13–51. 1994.

[2] José Valenciano and Robert G. Owens. An adaptive spectral element method for the one-dimensional Helmholtz equation. *Submitted.*

[3] J. Tinsley Oden, Abini Patra, and Yusheng Feng. An *h-p* adaptive strategy. *Adaptive, Multilevel, and Hierarchical Computational Strategies*, 157:23–47, 1992.

[4] J. Tinsley Oden, Weihan Wu, and Mark Ainsworth. An a posteriori error estimate for finite element approximations of the Navier-Stokes equations. *Computer Methods in Applied Mechanics and Engineering*, 111:185–202, 1994.

Unsteady Stokes Solvers for the Spectral/hp Element Methods.

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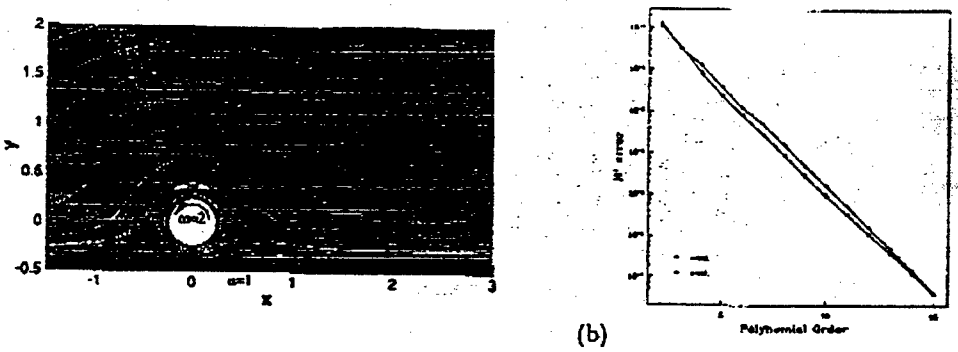

(a) (b)

Figure 1: (a) Iso-contours of vertical velocity and streamlines for Wannier-Stokes flow past a rotating cylinder. (b) Convergence as a function of polynomial order for the Wannier-Stokes problem.

Two very popular approaches to numerically solving the discrete incompressible Navier-Stokes equations are to either directly solve the matrix problem arising from the discretisation of the Stokes problem or to use a splitting/projection method where the velocity matrix system and pressure systems are typically decoupled.

The direct solution of the Stokes system introduces the problem of appropriate spaces for the velocity and pressure systems to satisfy the inf-sup condition [1] and requires the solution of the full velocity-pressure system. However, if a discontinuous pressure space is used then all but the constant mode of the pressure system can be decoupled from the velocity. Furthermore when implementing this approach with a spectral/hp element discretisation the remaining velocity system may then be statically condensed to decouple the so called interior elemental degrees of freedom, reducing the Stokes problem to a greatly reduced system expressed on the elemental boundaries [2, 3]. The direct solution of the Stokes problem provides a very natural setting for the solution of the pressure system which is not so easily dealt with in a splitting scheme. Further, the solution of the full coupled velocity systems means that the introduction of a spatially varying viscosity, which arise for example in non-Newtonian flows, is only a minor modification.

Splitting scheme are typically favoured for their numerically efficiency since for a Newtonian fluid the velocity and pressure systems are handled independently requiring the solution of three (in two-dimensions) elliptic systems of rank N as opposed to a single system of rank $3N$ solved in the Stokes problem. However, a drawback of this approach is the splitting error which is introduced when decoupling the pressure and velocity systems although this can be made consistent with the overall temporal accuracy of the scheme by appropriate discretisation of the pressure boundary conditions [4]. Although the pressure boundary conditions

are typically obtained in a consistent manner from the velocity system a discrepancy does arise when treating outflow boundaries where a constant Dirichlet value on pressure is applied otherwise numerical instabilities are experienced. Ideally the pressure at this boundary should be obtained directly from the velocity field as is the case in the direct Stokes solvers. A further complication of this scheme when using an iterative approach is the determination of an appropriate stopping criteria for the decoupled pressure and velocity systems.

Both of these approaches have been implemented within the framework of a Galerkin spectral/*hp* element method and it is the objective of this research to make a direct comparison of the two implementations in the context of unsteady Stokes problems. As shown in figure 1 both implementations have been validated for the steady Wannier-Stokes problems where exponential convergence to the steady state solution is achieved as a function of polynomial order. To develop an efficient unsteady Navier-Stokes solver a natural development to the present implementations is to consider the unsteady Stokes problem. However the matrix problems which arise from the discretisation of the Stokes problem have conditions numbers which grow with the spectral order of the spectral/*hp* element method and so there is a need for efficient preconditioners. It has been theoretically shown in [3] that for the steady stokes problem it is possible to reduce the growth of the condition number to a logarithmic function of spectral order divided by the inf-sup constant. We shall therefore be numerically and theoretically investigating a range of preconditioners including the use of block preconditioning and substructuring methods on the unsteady stokes problem as well as addressing the issue of element deformation.

References

[1] R. Stenberg and M. Suri. Mixed *hp* finite element methods for porblems in elasticity and Stokes flows. *Numer. Math.*, 72:367–389, 1996.

[2] P. Le Tallec and A. Patra. Non-overlapping domain decomposition methods for adaptive *hp* approximations of the Stokes problem with discontinuous pressure fields. *Comp. Meth. App. Mech. Engrg.*, 145:361–379, 1997.

[3] M. Ainsworth and S. Sherwin. Deomain decomposition preconditioners for p and *hp* finite element approximation of Stokes equations. *Comp. Meth. App. Mech. Engrg.* To appear.

[4] G.E. Karniadakis, M. Israeli, and S.A. Orszag. High-order splitting methods for the incompressible Navier-Stokes equations. *J. Comp. Phys.*, 97:414, 1991.

A high order splitting scheme for the Navier Stokes equations with variable viscosity.

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The use of Large Eddy Simulation and the desire to study non-Newtonian fluids, such as those which arise in biomedical fluid dynamics, require the ability to model the incompressible Navier-Stokes equation with a viscosity which may vary in both space and time, i.e.

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\nabla)\,\mathbf{V} = -\nabla \mathrm{p} + \nabla\cdot\left[\nu\left(\nabla\mathbf{V} + \nabla^{\mathrm{T}}\mathbf{V}\right)\right] \qquad \mathrm{Q} = \nabla\cdot\mathbf{V} = 0,$$

The introduction of a temporally and spatially varying viscosity means that the stress tensor cannot be simplified. The most straight forward approach to discretising the viscous term would be to treat it explicitly. This, however leads to undesirable time step restrictions, particularly in the spectral/*hp* method. The objective of this paper is, therefore, to construct a high-order time stepping scheme for the Navier Stokes equations with a semi-implicit treatment of the variable viscosity.

For a Galerkin implementation, it is advantageous to have a symmetric time independent viscosity and so we decompose the time dependent spatially varying viscosity $\nu(x,t)$ into two components $\nu = \nu_i + \nu_s$, where $\nu_i(x)$ is spatially varying, and will be treated semi-implicitly in time, while $\nu_s(x,t)$ is an instantaneous component and will be explicitly advanced in time. In order to decouple the velocity components, the linear term $L(\mathbf{V}) = \nabla\cdot\left[(\nu_i+\nu_s)\left(\nabla\mathbf{V}+\nabla^{\mathrm{T}}\mathbf{V}\right)\right]$, is split into $L(\mathbf{V}) = L^i(\mathbf{V}) + L^e(\mathbf{V})$, where $L^i(\mathbf{V}) = \nabla\cdot[\nu_i\nabla\mathbf{V}]$, is treated implicitly, and $L^e(\mathbf{V}) = \nabla\cdot\left[\nu_i\nabla^{\mathrm{T}}\mathbf{V}\right] + \nabla\cdot\left[\nu_s\cdot\left(\nabla\mathbf{V}+\nabla^{\mathrm{T}}\mathbf{V}\right)\right]$, is treated explicitly in a similar fashion to the non-linear term $N(\mathbf{V}) = (\mathbf{V}\cdot\nabla)\mathbf{V}$. We note that the explicit term $L^e(\mathbf{V})$ may be further manipulated using the divergence equation to reduce the differential order of the terms containing ∇^T.

Following the procedure from [1], a high order splitting scheme with spatially varying viscosity can be constructed, resulting into the three step solution process

$$\frac{\hat{\mathbf{V}}-\mathbf{V}^*}{\Delta t} = \sum_{q=0}^{J_e-1}\beta_q\left(-(\mathbf{V}\cdot\nabla)\mathbf{V} + (\nabla\nu_i)\left(\nabla^{\mathrm{T}}\mathbf{V}\right) + \nabla\cdot\nu_s\left(\nabla\mathbf{V}+\nabla^{\mathrm{T}}\mathbf{V}\right)\right)^{n-q} \tag{1}$$

$$\nabla^2 p^{n+1} = \nabla\cdot\left(\frac{\hat{\mathbf{V}}}{\Delta t}\right) + \nabla\cdot\sum_{q=0}^{J_i-1}\gamma_q\left[\nabla\cdot\nu_i\nabla\mathbf{V}\right]^{n+1-q} \tag{2}$$

$$\frac{\mathbf{V}^{n+1}-\hat{\mathbf{V}}}{\Delta t} = \sum_{q=0}^{J_s-1}\gamma_q\nabla\cdot\left[\nu_i\nabla\mathbf{V}\right]^{n+1-q} \tag{3}$$

where $\hat{\mathbf{V}} = \dot{\mathbf{V}} + \nabla p^{n+1}$ and the pressure equation is supplemented with the boundary condition

$$\frac{\partial p^{n+1}}{\partial \mathrm{n}} = \mathrm{n}\cdot\left[-\sum_{q=0}^{J_s-1}\beta_q\left[(\mathbf{V}\cdot\nabla)\mathbf{V} - (\nabla\nu_i)\nabla^{\mathrm{T}}\mathbf{V} - \nabla\cdot\nu_s(\nabla\mathbf{V}+\nabla^{\mathrm{T}}\mathbf{V})\right]^{n-q}\right] + \mathrm{n}\cdot\left[\sum_{q=0}^{J_i-1}\gamma_q\left[(\nabla\nu_i)(\nabla\mathbf{V}) - \nu_i\nabla\times(\nabla\times\mathbf{V})\right]^{n+1-q}\right] \tag{4}$$

We note that in equations (2) and (4), terms exist at time level $(n+1)$, leading to a coupled system. To decouple it, the linear terms are essentially consistently extrapolated from the previous time levels. Assuming $J_i = 2, \gamma_0 = 1-\theta, \gamma_1 = \theta$, equations (2),(3) and (4) can be

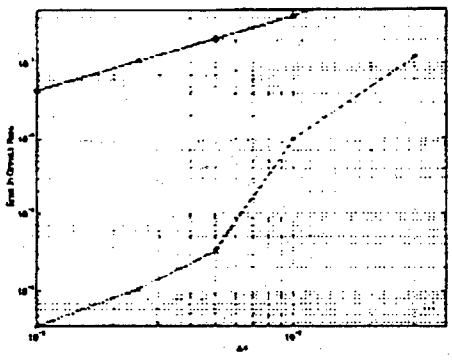

Figure 1: Error in decay-rate versus time step for the Stokes flow.

rewritten as

$$\nabla^2 p^{n+1} = \nabla \cdot \left(\frac{\hat{\mathbf{V}}}{\Delta t}\right) + \nabla \cdot \sum_{q=0}^{J_e-1} \beta_q \left[\nabla \cdot \nu_i \nabla \mathbf{V}\right]^{n+1-q} \tag{5}$$

$$\nabla \cdot \nu_i \nabla \mathbf{V}^* - \frac{1}{\Delta t(1-\theta)} \mathbf{V}^* = \frac{\hat{\mathbf{V}} + \frac{\theta}{1-\theta}\mathbf{V}^*}{\Delta t}, \mathbf{V}^* = (1-\theta)\mathbf{V}^{n+1} + \theta \mathbf{V}^n \tag{6}$$

$$\frac{\partial p^{n+1}}{\partial \mathbf{n}} = n \cdot \left[-\sum_{q=0}^{J_e-1} \beta_q \left[(\mathbf{V} \cdot \nabla)\mathbf{V} - (\nabla \nu_i)\nabla^{\mathrm{T}}\mathbf{V} - \nabla \cdot \nu_e(\nabla \mathbf{V} + \nabla^{\mathrm{T}}\mathbf{V})\right]^{n-q} \right] +$$

$$n \cdot \left[\sum_{q=0}^{J_e-1} \beta_q \left[(\nabla \nu_i)(\nabla \mathbf{V}) - \nu_i \nabla \times (\nabla \times \mathbf{V})\right]^{n-q} \right]. \tag{7}$$

The significant differences with the formulation for constant viscosity in [1] is the treatment of the viscous terms which requires the introduction of the extra expressions in the pressure equation and pressure boundary conditions in order to maintain a divergence free algorithm.

By using an implicit spatial viscosity and an explicit viscosity component such that the total viscosity is constant, the Stokes Channel flow and the Kovasznay flow were considered [1]. It has been shown that 2nd order temporal convergence is achieved. In Figure 1 we can see the error in decay-rate versus time time step for the Stokes channel flow, for a 3rd order Adams- Bashforth and Euler backward case (solid line) and 3rd order Adams- Bashforth and Crank-Nicholson (dotted line).

A full derivation of the above method will be presented, together with a numerical stability analysis of the decoupling of the viscous term. Further analytic solutions will be discussed as well as an application of the method in Large Eddy Simulation for a flow past a cylinder will conclude the paper.

References

[1] G.E. Karniadakis, M. Israeli, and S.A. Orszag. High-order splitting methods for incompressible Navier-Stokes equations. J. Comp. Phys., 97:414, 1991.

[2] G.E. Karniadakis, and S.J. Sherwin. Spectral/hp Element Methods for CFD, Oxford University Press.

[3] D.C. Leslie, and S. Gao. The Stability of Spectral Schemes for the Large Eddy simulation of Channel Flows. Int. Journal for Num. Methods in Fluids.,8:1107,1988.

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OPTIMAL APPROXIMATION OF SINGULARITIES BY NON-CONFORMING *hp* FINITE ELEMENT METHODS

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Abstract

Design over complex domains often requires the concatenation of separately constructed meshes over subdomains. Non-conforming elements are used to avoid the problem of coordinating the submeshes. Non-conforming techniques are also useful in applications where the discretization needs to be selectively increased in localized regions (such as those around corners or other features) which contribute most to the pollution error in any problem.

We address the stability and convergence of *hp* non-conforming methods, in particular, the mortar finite element method and some of its variants. We prove our methods are stable and optimal even when highly non-quasiuniform meshes are used to capture singularities. We also obtain estimates for the case that the polynomial degree is allowed to increase. In particular, we show that the exponential convergence obtained via conforming *hp* methods is preserved when the non-conforming mortar method is used.

Our estimates follow from the analysis of stability for an operator Π that arises in the matching at interfaces. We present numerical results that show these stability estimates to be sharp. In particular, the loss of a factor $k^{3/4}$ where k is the degree of polynomials used, cannot be

avoided in the stability estimates.

Our numerical results on an L-shaped domain with singular solution match well with the optimal h and hp convergence that our results predict. However, the loss of $k^{3/4}$ is not observable from the experiments, since the conforming and non-conforming cases behave almost identically.

Our results are primarily in two dimensions, but we briefly describe extensions to three dimensions as well. In particular, we define the mortar element method for arbitrary degree in three dimensions and give numerical evidence for the stability of the analogous operators II.

EFFECTS OF GEOMETRIC SINGULARITIES ON NAVIER-STOKES SOLUTIONS

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Abstract

In this presentation we will consider solutions of the incompressible Navier-Stokes in the presence of geometric singularities. In particular, we will analyze the primitive-variables formulation as well as the velocity-vorticity formulation, the latter being more sensitive to geometric discontinuities. The effect of such singularities on benchmark problems will be discussed and fixes will be proposed based on the auxilliary-mapping and singular-function techniques in the context of discontinuous Galerkin methods for elliptic equations.

Parallel Domain Decomposition for Reaction-Diffusion Problems

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Domain decomposition methods overlapping as well as non-overlapping ones have been studied for parabolic problems in works of Lions(1988),Rannacher (1994), Cai (1991), Kuznetsov(1990).

The purpose of this paper is to solve the three dimensional reaction- diffusion problem arising in the mathematical modeling of calcium dynamic in the neurons. The solution of the problem necessitates very large 3D meshes due to its geometric complexity. A domain decomposition strategy was selected to overcome this and the large time intervals resulting from the original problem. A Schwarz alternative method was applied to the nonlinear problem and a number of smaller nonlinear problems were solved per domain decomposition iteration. Inside each subdomain we used we used the standard FEM package, FIDAP (Engelman,1993) which was modified for PVM (Geist et al., 1994) parallelization (Aharon et al., 1996) and was supplemented by the options of time management introduced in (Bercovier et al., 1997). The computations we performed on SP2 machine.

The actual reaction-diffusion problem is :

Consider a bounded domain, Ω of R^3 such that $\partial\Omega$ is its boundary. Then, the full problem we want to solve is the following :
Find u_i (i =1,..n), the real valued functions, defined on Ω and satisfying :

$$\begin{cases} \partial_t u_i - \nu_i \triangle u_i = \partial_t f_i \quad \text{in} \quad \Omega \times (0,T] \\ \partial_t f_i = \sum_{j=1}^{n} (-\lambda_j u_i u_j + \mu_j u_{ij}) \quad \text{in} \quad \Omega \times (0,T] \\ \partial_n u_i = g_i \quad \text{on} \quad \partial\Omega \times (0,T] \\ u_i|_{t=0} = u_{i0} \quad \text{in} \quad \Omega. \end{cases} \tag{1}$$

Above u_i is the concentration of the i component of the system, ν_i is the corresponding diffusion coefficient, $\partial_t f_i$ denotes the reaction of the i component with others of the system, where λ_{ij} and μ_{ij} are the rate constants and u_{ij} is the binding complex of i and j component.

The present domain decomposition method uses over-lapping non necessarily "mesh consistent" geometries. Thus we can treat several geometric scales at the same time. (Aharon at all, 1996) We define the domain decomposition iterations not on each time step of computation but on automatically determined common times for updating the individual subdomains boundary

conditions. These global time points are an essential parameter for the the algorithm optimization. Such an approach provides not only different space but also different time resolution on each subdomain.

Numerical tests of the algorithm were undertaken. It took about several days to calculate the described here general problem without parallel domain decomposition on an Indy SGI workstation. Parallel computations on a SP2 machine gave us the results in hours. The algorithm presented here is fully parallel relative to the number of domains , that is the total solution time is the same whether for 4 domains on 4 processor or 32 domains on 32 processors.

ND	NODF	RT	UT
32	12 804	5 940	143 880
16	20 976	11 520	141 600
8	41 268	24 240	138 240

Table 1: Reaction- diffusion problem was solved for domain with 32 spines. DD algorithm was applied for partition on 32, 16 and 8 domains. ND - number of domains. NODF - number of degrees of freedom. RT - real time of computation in sec. UT - user time(sec) - total time of computation.

References

[1] Aharon, S., Bercovier, M., Parnas,(1996) H.Parallel computation enables precise description of Ca^{2+} distribution in nerve terminals. Bull. Math. Biol. 58:1075-1099

[2] Bercovier, M, N Volfovsky and Parnas.(1997) Parallel Domain Decomposition for Reaction-Diffusion Problems. "Computational Science for the 21st century". Conference in honor of Professor R. Glowinski. May5-7,1997.

[3] Cai X,-C.(1991) Additive Schwarz algorithm for parabolic convection-diffusion equations Numer. Math. 60:41 -61

[4] Engelman M.S. (1993) FIDAP Theoretical Manual,version 7.0. *FDI,Evanston,IL*

[5] Kuznezov Y.A. (1990)Domain decomposition methods for unsteady convection-diffusion problems,*proc . 9th Int Conf on Comput.Meth. Appl. Sci. Engin.(Glowinski and Lions, eds., SIAM, Philadelphia*

[6] Lions, P.L. (1988) On the Schwarz alternating method. I. In: R. Glowinski, G.H. Golub, G.A. Meurant, J. Périaux eds., First International Symposium on Domain Decomposition Methods for Partial Differential Equations, SIAM, Philadelphia.

[7] R. Rannacher R.(1994) Domain decomposition in the nonstationary streamline diffusion finite element method*Proc FEM 50 Fifty Years Finite Element Method, Javakyla, September 1993 (P. Neitaanmaki, ed.)*

Stable and unstable formulations of the convective terms in spectral element simulations

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The effects on stability of the formulation of the nonlinear terms $(\underline{u} \cdot \nabla)\underline{u}$ in the incompressible Navier-Stokes equations are examined in the context of spectral element methods. For single-domain spectral methods the influence of the different formulations has been studied in detail (see e.g. Canuto et al., 1988), but much less work has been devoted to this issue for spectral element methods. In our work, we use the $P_N - P_{N-2}$ method (see e.g. Fischer, 1997), where the velocities and the pressure are discretized at the Gauss-Lobatto-Legendre (GLL) points and at the Gauss-Legendre (GL) points, respectively. For the temporal discretization two different mixed implicit/explicit schemes have been implemented. The first is a combination of a Crank-Nicolson scheme for the viscous terms and a third-order Adams-Bashforth scheme for the nonlinear terms (CN/AB3). The second method combines the third-order backward-differentiation scheme for the viscous terms with a third-order extrapolation scheme for the nonlinear terms (BDF3/EX3).

We have compared four different (but mathematically equivalent) formulations of the nonlinear terms, namely the *convective form* $\underline{N} = (\underline{u} \cdot \nabla)\,\underline{u}$, the *divergence form* $\underline{N} = \mathrm{div}\,(\underline{u} \otimes \underline{u})$, the *skew-symmetric form* $\underline{N} = 1/2\,(\underline{u} \cdot \nabla)\,\underline{u} + 1/2\,\mathrm{div}(\underline{u} \otimes \underline{u})$, and the *rotational form* $\underline{N} = -(\underline{u} \times \underline{\omega}) + 1/2\,\mathrm{grad}|\underline{u}|^2$ (here $\underline{u} \otimes \underline{v}$ denotes the tensor product of $\underline{u}$ with $\underline{v}$, and $\underline{\omega} = \mathrm{rot}\,\underline{u}$). For the convective form, the divergence form and the skew-symmetric form the derivatives of the velocity are computed at the GLL points. For the rotational form, the term $1/2\,\mathrm{grad}|\underline{u}|^2$ can either be added to the pressure and evaluated at the GL points or the term can by computed at the GLL points. The first variant is denoted as "*rot*1" and the second as "*rot*2".

As a test case, we studied the temporal two-dimensional Orr-Sommerfeld problem for plane Poiseuille flow with no-slip boundary conditions at the walls and periodicity in the streamwise direction. The simulation was initialized with the laminar Poiseuille profile and a superimposed Tollmien-Schlichting wave of amplitude 10^{-4}. The Reynolds number based on channel half-width and centerline velocity was $Re = 7500$. Figure 1 compares the temporal evolution of the respective perturbation energies for the different formulations of the nonlinear terms. It is readily seen that only the convective form and the rotational form *rot*2 are stable, while all other formulations are unstable and lead to blow-up within one period $T_{TS} \approx 25$ (stability was confirmed up to $t = 40\,T_{TS}$).

We have analyzed this instability with respect to its dependence on the temporal and spatial resolution, the time discretization scheme, the Reynolds number of the flow, and the boundary conditions imposed. Specifically, we found the results to be essentially identical for the BDF3/EX3 and the CN/AB3 schemes. Also, the time step, the number of elements and the polynomial degree on each element were found to have no effect on the general stability properties, but resulted in quantitive differences only. (Of course, the time step was always chosen well below the CFL stability limits of the EX3 and AB3 schemes, respectively.) We can also exclude that the stability problem originates from the treatment of the periodic boundaries in the streamwise direction. We have conducted simulations where the periodic boundary conditions were replaced by Dirichlet conditions taken from the linear eigensolution, and encountered the same instability. Only for sufficiently low Reynolds numbers (below 100) the schemes remain stable, irrespectively of the treatment

of the nonlinear terms, obviously due the viscous diffusion.

In the unstable cases the amplitude of the disturbance grows exponentially with time. We suppose that the instability is linked to the use of a staggered grid. An eigenvalue analysis of the spatial discretization operator for a simple scalar convection equation does not show significant differences between the (stable) convective form and the (unstable) divergence form. It is interesting to note that we found the skew-symmetric form to be unstable, while other investigations (e.g. Rønquist, 1996) suggested that it should be the preferred choice. For a more in-depth analysis of the stability problem we are currently performing an eigenvalue analysis of the fully discretized system.

References

P. F. Fischer (1997), An Overlapping Schwarz Method for Spectral Element Solution of the Incompressible Navier-Stokes Equations *J. Comput. Phys.*, Vol.133, pp. 84-101

C. Canuto, M.Y. Hussaini, A. Quateroni, T. A. Zang (1988), Spectral Methods in Fluid Dynamics, Springer, Berlin

E. M. Rønquist (1996), Convection Treatment Using Spectral Elements of Different Order *Int. J. Numer. Methods Fluids*, Vol. 22, pp. 241-264

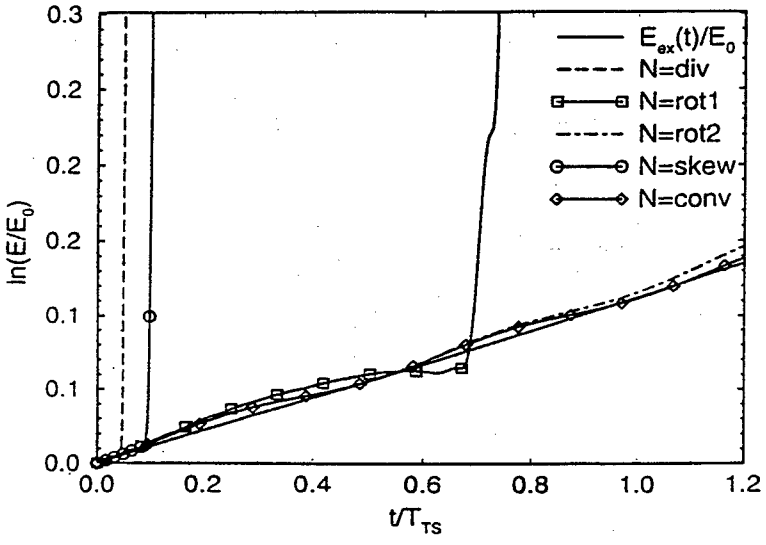

Figure 1: Perturbation energy $E(t)$ for the Orr-Sommerfeld test case computed with different formulations of the nonlinear terms (convective, divergence, rotational and skew-symmetric forms). For comparison the exact perturbation energy $E(t) = E_o\, e^{2\omega_i t}$ is included. Computation with 2×4 spectral elements with polynomial degree of $N = 12$ in each element and each direction. Temporal discretization with CN/AB3 scheme with $\Delta t = 0.01 \approx 4 \cdot 10^{-4}\, T_{TS}$.

An Optimal Mesh Choice for the (σ, θ)-methods[1]

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Abstract of the paper

In this paper we consider the one-dimensional heat conduction equation. The so-called (σ, θ)-method will be applied to the numerical solution of the problem. The (σ, θ)-method unites a few numerical methods. With the choice $\sigma = 0$ we get the finite difference θ-method and the choice $\sigma = 1/6$ results in the finite element Galerkin-method with linear elements. The most important question in the numerical solution is the choice of the suitable mesh-parameters (τ, h). The basic condition comes from the condition of the convergence. Moreover, it is reasonable to choose such a convergent numerical method which is optimal in a certain sense. We define the optimal method as follows. The fixed number $T \in \mathbb{R}^+$ denotes the time level at which the global error will be minimized and $M \in \mathbb{N}$ denotes the number of the arithmetic operations (multiplications and additions) used for the determination of the numerical solution at the time level T. Let us denote the approximation of the exact solution at the time level T obtained by the (σ, θ)-method with the help of M operations by $\mathbf{y}^{T,M}$. Denoting the exact solution at the time level T at the mesh-points by $\mathbf{u}^T$, we set $z^{T,M} = \| \mathbf{u}^T - \mathbf{y}^{T,M} \|_{l_2}$.

DEFINITION. *Let T, M, $\sigma \in [0, \frac{1}{4})$ and $\theta \in [0, 1]$ be fixed numbers. We say that the mesh with mesh-parameters h_{opt}, τ_{opt} is optimal if the error $z^{T,M}$ is minimal on this mesh.*

The solution of the continuous problem has several qualitative properties. Some of them are the following: contractivity in maximum norm, suitable convergence in time, preservation of nonnegativity and shape of the initial function, etc. They characterize qualitatively the heat conduction process. It is not less important to draw up the qualitative properties in the numerical case, and to examine their conditions. For any (σ, θ)-method these conditions result in upper bounds for the parameter $\frac{\tau}{h^2}$ (that is for the choice of the mesh), even for unconditionally stable schemes, too. The preservation of the nonnegativity plays a fundamental role since it implies the preservation of the most important qualitative properties. Therefore, we examine only the preservation of nonnegativity. We say that the numerical method preserves the nonnegativity if the condition $\mathbf{y}^0 \geq 0$ implies $\mathbf{y}^j \geq 0$ for all $j = 1, 2, \ldots$. Here the vector $\mathbf{y}^j$ denotes the approximation of the exact solution at the time level $j \cdot \tau$.

We compare our optimal parameters with the bounds obtained for the preservation of basic qualitative properties. As a result, we obtain the parameter choice

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for any convergent method being both optimal and preserving the main qualitative properties.

LEMMA. *The (σ,θ)-methods with $(\theta-\frac{1}{2})(\frac{1}{12}-\sigma)<0$ preserve the nonnegativity on the optimal mesh if and only if the value θ is between the values $\frac{6\sigma+2}{5}$ and 6σ.*
The (σ,θ)-methods with $(\theta-\frac{1}{2})(\frac{1}{12}-\sigma)>0$ preserve the nonnegativity on the optimal mesh if and only if the condition

$$\frac{\sigma}{\theta}\le\sqrt[3]{\frac{125}{13}}\cdot\frac{1-12\sigma}{12\theta-6}\le\frac{\frac{1}{2}-\sigma}{1-\theta},\qquad\theta\ge 2\sigma$$

is fulfilled.
The $(\frac{1}{12},\frac{1}{2})$-method preserves the nonnegativity on the optimal mesh.

It is known that the explicit methods work with less arithmetic operations than the implicit ones. According this fact we can increase the accuracy. In this paper we suggest that explicit methods or methods with higher order will be used. The best methods are the $(\sigma,6\sigma)$-methods which have higher order and are explicit simultaneously. We remark that these methods are equivalent because they yield the same iteration process.

Finally, numerical examples are given. The examples show that the computed, optimal parameters are optimal indeed, even for non-continuous initial functions. For example, let us consider the heat equation with initial function $u_0(x)=sin(\pi x)$. Then the exact solution is $u(x,t)=sin(\pi x)e^{-\pi^2 t}$. Let the time level be $T=0.1$ and let the number of operations be $M=10^6$. The different (σ,θ)-methods are compared in the table below.

method	h_{opt}	τ_{opt}	l_2-error
$(0,0)$	1.4286×10^{-2}	3.41×10^{-5}	2.3361×10^{-10}
$(1/12,1/2)$	1.4972×10^{-2}	8.68×10^{-5}	1.2799×10^{-9}
$(1/6,2/3)$	1.3699×10^{-2}	9.25×10^{-5}	6.8118×10^{-8}
$(1/20,2/3)$	1.0989×10^{-2}	11.6×10^{-5}	6.2782×10^{-6}

It can be seen that he $(0,0)$-method has higher order and is explicit realizing the most accurate method.

References

[1] Samarskii, A.A. *Theory of the difference schemes, Nauka, Moscow, 1977.*

[2] Faragó, I., One-step Methods of Solving a Parabolic Problem and their Qualitative Properties, Publications on Applied Analysis, Eötvös L. University, Department of Applied Analysis, Budapest, 1996/3

[3] Laurie, D.P. *Optimal parameter choice in the θ-method for parabolic equations, J. Inst. Maths Applics, 19 (1977), 119-125.*

[4] Scott, J.A., Seward, W.L. *Finite difference methods for parabolic problems with non-smooth initial data, Oxford University Computing Laboratory, Numerical Analysis Group, Report Number 86/22, 1987.*

[5] Faragó, I., Horváth R., *An Optimal Mesh Choice in the Numerical Solution of the Heat Equation, Computers and Mathematics with Applications*

[6] Horváth, R. *On the positivity of iterative methods, Annales Univ. Budapest. Sect. Comp., Budapest, 1995, to appear.*

[7] Faragó, I., On the Non-negative Solution of Some System of Linear Algebraic Equations and its Application to the Numerical Solution of Partial Differential Equations, Quaderni del Dipartimento di matematica, Statistica, Informatica e Applicazioni, Bergamo (1992).

[8] Faragó, I. *Nonnegativity of the difference schemes, Pure Math. Appl., 6 (1996), 38-50.*

[9] Faragó, I. *Qualitative properties of the numerical solution of linear parabolic problems with nonhomogeneous boundary conditions, Computers Math. Applic., 31 (1996), 143-150.*

Legendre Spectral Collocation for the Biharmonic Dirichlet Problem

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Abstract

We consider a spectral collocation method for the solution of the biharmonic Dirichlet problem:

$$\Delta^2 u = f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega,$$

where Δ denotes the Laplacian, $\Omega = (-1,1)\times(-1,1)$, $\partial\Omega$ is the boundary of Ω, and $\partial/\partial n$ is the outer normal derivative on $\partial\Omega$. Recently, efficient spectral Galerkin methods, which are based on the standard variational formulation of the problem, have been considered in [1], [2], and [3]. In this paper, following the approach of Ciarlet and Raviart, we introducing $v = \Delta u$ to obtain the coupled problem

$$-\Delta u + v = 0 \text{ in } \Omega, \quad -\Delta v = -f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega.$$

Let P_N, where $N \geq 4$, be the set of polynomials of degree $\leq N$ on $(-1,1)$ and let

$$P_N^0 = \{p \in P_N : p(\pm 1) = 0\}, \quad P_N^{00} = \{p \in P_N^0 : p'(\pm 1) = 0\}.$$

Let $\{\xi_i\}_{i=1}^{N-1}$ be the nodes of the $N-1$-point Gauss-Legendre quadrature on $(-1,1)$. Our spectral collocation problem consists in finding $U \in P_N^{00} \otimes P_N^{00}$ and $V \in P_N \otimes P_N$ such that

$$-\Delta U(\xi_i,\xi_j)+V(\xi_i,\xi_j) = 0, \quad -\Delta V(\xi_i,\xi_j) = -f(\xi_i,\xi_j), \quad i,j = 1,\ldots,N-1,$$

and

$$V(a,b) = V_y(a,b) = 0, \quad a,b = \pm 1.$$

We prove existence and uniqueness of the collocation solution and establish error bounds in Sobolev norms. The matrix-vector form of the spectral collocation problem is derived using basis functions of [2] for the spaces P_N^0 and P_N^{00}. These functions are linear combinations of two and three Legendre polynomials, respectively. We use a Schur complement approach to reduce the resulting linear system to a linear system involving the approximation V of v on the two vertical sides of Ω. The Schur complement system is set up by solving an auxiliary collocation problem for a related biharmonic problem with Δu instead of $\partial u/\partial n$ specified on the two vertical sides of Ω. The auxiliary collocation problem is solved using a matrix decomposition algorithm which involves the solution of two symmetric eigenvalue problems with tridiagonal matrices. The Schur complement system is solved by a Gauss elimination method. Once the approximation to v on the vertical sides is obtained, approximations to v and u in Ω are computed. The total cost of the algorithm is $O(N^3)$. Numerical results demonstrate spectral convergence of the method.

[1] P.E Bjørstad and B.P. Tjøstheim, *Efficient algorithms for solving a fourth-order equation with the spectral-Galerkin method*, SIAM J. Sci. Comput., 18 (1997), 621–632.

[2] J. Shen, *Efficient spectral-Galerkin method I. Direct solvers of second- and forth-order equations using Legendre polynomials*, SIAM J. Sci. Comput., 15 (1994), 1489–1505.

[3] J. Shen, *Efficient spectral-Galerkin method II. Direct solvers of second- and forth-order equations using Chebyshev polynomials*, SIAM J. Sci. Comput., 16 (1995), 74–87.

A Spectral Collocation Time-Domain Method for Diffractive Optics

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Diffractive Optical Elements (DOEs) employing surface-relief gratings on planar optical waveguides have become increasingly interesting for sensor applications as the fabrication technology for such devices has matured. At the same time, the actual specification of the surface modulation remains a significant challenge. Since the structures contains sub-wavelengths variations, analytic tools are clearly insufficient, and also low-order numerical schemes such as the Finite Difference Method will in most cases fail to reproduce details of the out-of-plane coupled optical field. This is due to the fact that such methods do no accurately model the phase behaviour of the field as it propagates in the structure. Since the structure will typically be hundreds of wavelengths long, phase errors will accumulate and lead to unreliable solutions for the out-coupled wavefronts

We present a spectral method for modeling optical waveguide structures comprising surface relief gratings for out-of-plane out- or in-coupling of light. A similar scheme has previously been employed in the calculation of electromagnetic scattering from conducting surfaces [2].

The starting point for our analysis is the time-domain Maxwell equations. In the 2D case, TE- and TM-modes exist and we shall restrict our analysis to TE-modes. We set up a computational framework involving the combination of a number of techniques which together form a strong and flexible tool for modelling wave propagation in geometrically complex structures.

The key issue in the development presented here is the accurate spatial approximation. The equations are advanced in time using a low-storage 5-stage 4th-order- Runge-Kutta scheme [2].

The core of the numerical algorithm is a Chebyshev collocation scheme with its superior approximation properties. This scheme is used to estimate the first order spatial derivates in the Maxwell equations on the cosine distributed Chebyshev-Gauss-Lobatto grid points. We employ a weak Super-Gaussian filtering of the solution which is found to increase the robustness of the scheme.

In order to derive a geometrically flexible scheme, where the grid need not be rectangular, we use transfinite linear blending functions [3] to smoothly map a general quadrilateral to the unit square. The Maxwell equations must then be expressed in general curvilinear coordinates.

As the time-domain Maxwell equations form a set of hyperbolic partial differential equations, we can take advantage of the characteristic variables of such a system to extend our problem to a multi-domain formulation. For each time-step, a local solution is first found in each sub-domain. The characteristic variables are then subsequently used to patch the local solutions from each sub-domain to form the global solution for the entire computation domain. On boundaries between sub-domains of different refractive indices, we rigorously employ the physical boundary conditions, whereas at outer boundaries we introduce Perfectly Matched Layers [4].

Using this multi-domain formulation where each sub-domain can be a general quadrilateral, we achieve a great flexibility with respect to the geometry of the waveguide structure, and we are thus able to model wave propagation in diffractive optical elements with even very complex surface modulation.

As an important post-processing step, we must be able to calculate the out-coupled field in any distance from the waveguide structure. Here, integration techniques to perform both near- and farfield transformations of the out-coupled wavefront are used. In this way, the computation domain need only be extended to slightly above the waveguide structure where a synthetic aperture is placed. Equivalent electric and magnetic currents are then calculated on this aperture, and from these currents, the field anywhere above the aperture can be calculated rigorously. We employ methods for direct calculation of the field components in any distance as well as for calculation of farfield radiation patterns.

References

[1] B. Yang, D. Gottlieb, and J. S. Hesthaven, *Spectral Simulation of Elec-*

tromagnetic Wave Scattering, J. Comput. Phys. **134 (1997), pp. 526-534.**

[2] M. H. Carpenter and C. A. Kennedy, *Fourth-Order 2N-Storage Runge-Kutta Schemes, NASA-TM-109112, 1994*

[3] W. Gordon and C. A. Hall, *Transfinite Element Methods: Blending-Function Interpolation over Arbitrary Curved Element Domains, Numer. Math.* **21 (1973), pp. 109-129.**

[4] J. P. Berenger, *A Perfectly Matched Layer for the Absorption of Electromagnetic Waves, J. Comput. Phys.* **114 (1994), pp. 185-200.**

Spectral Method for Supersonic Compressible Flow Simulations.

by Wai-Sun Don

Abstract for ICOSAHOM 98

Spectral (Collocation) method, well known for its superior accuracy of smooth solution of the nonlinear partial differential equations, does not perform as well for discontinuous solutions.
Prime examples are the Burgers' equation and supersonic compressible Navier Stokes flow.

In contrast to general believes Gibbs phenomenon, associated with discontinuous functions, does not pose any difficult for spectral methods for the solution of nonlinear PDE.
The main causes of difficulty in obtaining both the temporal and spatial accuracy for such cases are the nonlinear instability and insufficient resolution for resolving the fine scale structures of the shocked flow.

The advance shock capturing high order finite difference schemes such as ENO, WENO and FCT, applied the necessary amount of numerical viscosity near hydrodynamic discontinuities for the removal of Gibbs in order to obtain a stable solution and at the same time retaining high accuracy within smooth regions.
On the other hands, Spectral methods requires an explicit mechanism, namely filter, to maintain stability for the numerical evolution of the nonlinear PDE.
It had been shown (Vandeven) that spectral accuracy can be achieved away from the discontinuity.

With the advent of computing capability of both vector and parallel computer, larger number of grid points (polynomials) can be taken to better resolve the flow fields with shock and fine scale structures.
However, larger number of grid points (N) does not necessary translate directly into better solution and/or efficient algorithm.
Roundoff error becomes a dominant source of errors resulting a worst solution as N increases.
Moreover, restrictive time step for stability of the discretized PDE using explicitly time stepping schemes becomes a major issue for efficiency.
These issues will be addressed and resolved through the use of mapping derived by Kosloff and Tal-Ezar.

One of the main computational kernels in the solution of the PDE using collocation methods is the differentiation operator.
As the number of grid points (polynomials) becomes increasingly large (N>64), issues related to its numerical implementation such as roundoff error and efficiency become very important.
Given the number of potential numerical algorithm (Matrix Multiply, Fast Fourier Transform etc.) and computational architecture available (CRAY, SGI, IBM SP2 etc.), an optimized and efficient software library is solely needed.
We will briefly describe the major components and capabilities of an existing library PseudoPack.
Issues related to parallel algorithms on distributed memory machine would also be discussed.

Results from the supersonic combustion and compressible mixing Layer simulations will be presented to demonstrate the capability of the spectral methods in capturing fine scale structures even for shocked flow.

Structural Acoustics Analysis Using Geometry-based p-version Finite and Infinite Elements

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Abstract

We present a computational framework that combines the superior approximation properties of variable-order, p-version finite and infinite elements with exactly mapped element geometries for highly accurate numerical solutions of coupled structural acoustics problems. The geometry of the (visco)elastic scatterers or radiators is three-dimensional. They may be fluid-filled or evacuated, and are considered to be submerged in an infinite acoustic medium.

The strong form of the governing partial differential equations is given by

$$\sigma_{ij,j}(u) + \rho_s\omega^2 u_i = 0 \text{ in } \Omega_s, \quad (1)$$

$$\sigma_{ij}(u)n_j = t_i^- \text{ on } \Gamma_-, \quad (2)$$

$$\sigma_{ij}(u)n_j = t_i^+ - \phi n_i \text{ on } \Gamma_+, \quad (3)$$

$$\Delta\phi + k^2\phi = 0 \text{ in } \Omega_+, \quad (4)$$

$$\frac{\partial\phi}{\partial n} = -\rho_f\omega^2 u_i n_i \text{ on } \Gamma_+, \quad (5)$$

$$\lim_{r\to\infty} r(\frac{\partial\phi_s}{\partial r} - ik\phi_s) = 0, \quad (6)$$

where Ω_s and Ω_+ denote the structural and infinite acoustic domains; Γ_- and Γ_+ denote the interior and exterior boundaries of the structure; n denotes the unit normal on Γ_- and Γ_+ directed out of the structure; u and σ_{ij} denote the elastic displacement field and stress tensor; ϕ and ϕ_s denote the total and scattered acoustic pressures; ρ_s and ρ_f

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denote the densities of the elastic and acoustic media; $k = \frac{\omega}{c}$ denotes the acoustic wavenumber where ω is the circular frequency and c is the sound speed.

The infinite domain is truncated by a prolate spheroid and discretized using infinite elements with *a-priori* satisfaction of the *Sommerfeld* condition given by equation (6). The resulting finite acoustic and the structural domains are discretized using unstructured, conforming finite elements. The piecewise polynomial approximation bases used for the finite and infinite elements are p-hierarchic and admit variable polynomial order within the closure of individual elements to allow for possible non-uniform p-adaptivity. The element geometric mapping is based on blending the exact mathematical description of the domain geometry housed within a CAD system. This preserves the exponential rate of solution convergence offered by the p-version finite and infinite elements.

Examples involving complex three-dimensional geometries show the ability of the framework to compute accurate solutions for acoustic radiation and scattering problems.

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NOVEL SPECTRAL AND FINITE ELEMENT METHODS FOR TRANSIENT PROBLEMS

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ABSTRACT

Finite element procedures for time dependent problems traditionally involve two stages. The continuum is discretized into finite elements. This leads to sets of ordinary differential equations which are then integrated numerically by classical schemes (e.g. Runge-Kutta, predictor-corrector, finite differences, etc.).

The solution method chosen in this work is the spectral element method. This is a high-order weighted residual method which exploits the rapid convergence rates of spectral methods while retaining the geometric flexibility of the low-order isoparametric finite element methods.

Semi-discrete spectral element algorithms have been developed for the simulation of unsteady incompressible fluid flow and heat transfer[1]. This semi-discrete approach is of high-order accuracy in space but only of low-order accuracy in time and, therefore, the error of the fully discretized method is dominated by the temporal error.

Spectral methods become very attractive because the correct pattern of the flow and its critical parameters can be obtained with relatively few numbers of base functions[2-4]. However, high temporal discretization is required for obtaining accurate numerical simulation of unsteady flow structures in the regions of parameter space, where oscillatory and chaotic flow structures are possible[2-4]. This leads naturally to the study of an important class of time and space-time spectral element methods.

The concept of applying time and space-time finite element approximations was pioneered in the late sixties and since then has been expanded and further developed through discontinuous spatial and temporal discretizations ([5]-[10] and references therein).

This paper deals with the formulation, implementation, and application of potentially powerful temporal and spatial spectral element approximations for solving initial and initial-boundary value problems. Point collocation, subdomain collocation, least squares, continuous and discontinuous Galerkin methods are analyzed and their characteristics in terms of accuracy and stability are presented and discussed. An adaptive time spectral element methodology is developed for Lagrangian spectral elements and its computational performance is demonstrated for stiff systems of ordinary differential equations appearing in dynamical systems[7,10], in chemical reactions[11] and in nonlinear control[12-13]. Space-time spectral element methods are presented and used to solve the transient diffusion of mass and energy equations in a spherical catalyst pellet with an exothermic reaction[14].

REFERENCES

1. Maday, Y., Patera, A.T. and Ronquist, E.M., An Operator-Integration-Factor Splitting Method for Time-Dependent Problems: Application to Incompressible Fluid Flow, *Journal of Scientific Computing*, Vol. 5, pp 263-292, 1990.

2. Bar-Yoseph, P., On Multiple Flow Patterns and Vortex Breakdown Phenomena in Confined Rotating Flows, *Computational Fluid Dynamics Journal*, Vol. 3, No. 3, pp 273-292, 1994.

3. Gelfgat, A.Y., Bar-Yoseph, P.Z. and Solan, A., Stability of Confined Swirling Flow with and without Vortex Breakdown, *Journal of Fluid Mechanics*, Vol. 311, pp 1-36, 1996.

4. Gelfgat, A.Y., Bar-Yoseph, P.Z. and Yarin, A.L., On Oscillatory Instability of Convective Flows at Low Prandtl Number, *ASME Trans., J. Fluids Eng.* (to appear in 1998).

5. Bar-Yoseph, P., Space-Time Discontinuous Finite Element Approximations for Multi-Dimensional Nonlinear Hyperbolic Systems, *Computational Mechanics*, Vol. 5, pp 145-160, 1989.

6. Bar-Yoseph, P. and Elata, D., An Efficient L2 Galerkin Finite Element Method for Multi-Dimensional Nonlinear Hyperbolic Systems, *Int. J. Numer. Methods Eng.*, Vol. 29, pp 1229-1245, 1990.

7. Aharoni, D. and Bar-Yoseph, P., Mixed Finite Element Formulations in the Time Domain for Solution of Dynamic Problems, *Computational Mechanics*, Vol. 9, pp 359-374, 1992.

8. Bar-Yoseph, P., Moses, E., Zrahia, U. and Yarin, A.L., Space-Time Spectral Element Methods for One-Dimensional Nonlinear Advection-Diffusion Problems, *J. Comput. Phys.*, Vol. 119, pp 62-74, 1995.

9. Bar-Yoseph, P.Z. and Moses, E., Space-Time Spectral Element Methods for Unsteady Convection-Diffusion Equations, *Int. J. Numer. Methods Heat & Fluid Flow*, Vol. 7, pp 215-235, 1997.

10. Bar-Yoseph, P.Z., Fisher, D. and Gottlieb, O., Spectral Element Methods for Nonlinear Spatio-Temporal Dynamics of an Euler-Bernoulli Beam, *Computational Mechanics*, Vol. 19, pp 136-151, 1996.

11. Finlayson, B.A., *Nonlinear Analysis in Chemical Engineering*, McGraw-Hill, New York, 1980.

12. Ben-Tal, A., Bar-Yoseph, P.Z. and Flashner, H., Space-Time Spectral Element Method for Optimal Slewing of a Flexible Beam, *Int. J. Numer. Methods Eng.*, Vol. 39, pp 3101-3121, 1996.

13. Naveh, Y., Bar-Yoseph, P.Z. and Halevi, Y., "Time Spectral Element Modeling and Control of Unicycle", submitted to the Fourth World Congress on Computational Mechanics, to be held in Buenos Aires, 29 June - 2nd July, 1998.

14. McGuire, M.L. and Lapidus. L., On the Stability of a Detailed Packed-Bed Reactor. *A.I.Ch.E. J.*, Vol. 11, pp 85-95, 1965.

An Efficiency Element-by-Element Preconditioner for Elliptic Boundary Value Problems*

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Today, robust and efficient parallel algorithms for solving the linear system of equations resulting from large-scale problems of engineering, physics, chemistry, computer science, mathematics and medicine, whose rate of convergence is optimal or nearly optimal and is independent of both jumps of coefficients and anisotropy, are of considerable importance. Recently the variable-step multilevel preconditioning method for self-adjoint and positive definite elliptic problems, discretized by the finite element method, have been proposed [3]. In spite of the fact that its rate of convergence is limited by that of the exact hierarchical two-level method [1, 6], it is robust in the above sense and, in addition, has the advantage of being totally free of parameters to estimate as well as robust with respect to the regularity of the elliptic problem. However, this method has the same disadvantage as the algebraic multilevel or multigrid methods, in the respect that to get an optimal order both of the rate of convergence and of the arithmetical cost per iteration these methods require the number of nodes on the initial (coarse) grid to be sufficiently small assuming that we solve this system by a direct method. A similar requirement holds if we solve it by an element-by-element method. The latter can be a great problem in their application for solving real life problems, since in order to obtain a good approximation we have to use a large number of levels. On the other hand, when solving extremely large-scale problems, for example of the order 100M - 1000M ($10^8 - 10^9$ degrees

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of freedom), i.e., where the full matrix data structure cannot be located in a single memory, there is a problem of assigning or distributing data among processors. One possible way to solve it is to keep the matrices in the element level form, i.e., the original matrix and its preconditioner are not based on the global stiffness matrix.

In the present talk a simple and efficient way to overcome these difficulties is suggested. By the combination of the new, generalized conjugate gradient method with a variable-step preconditioner [2, 3], and the old, element-by-element preconditioned conjugate gradient (EBE/PCG) method [4, 5], techniques we obtain an element-by-element version of the variable-step multilevel preconditioning method, which is nearly (asymptotically) optimal and in which both the original matrix and its preconditioner are stored as a set of elementary finite element stiffness matrices and their preconditioners. Note that the use of the proposed method for parallel computers is very natural since all required operations are additive and we use the local finite element data structure only.

References

[1] O. Axelsson, I. Gustafsson, *Preconditioning and two–level multigrid methods of arbitrary degree of approximation*, Math.Comp., 40 (1983), pp. 219–242.

[2] O. Axelsson, P. Vassilevski, *A black box generalized conjugate gradient solver with inner iterations and variable–step preconditioning*, SIAM J.Matrix Anal. Appl., 12 (1991), pp. 625–644.

[3] O. Axelsson, P. Vassilevski, *Variable–step multilevel preconditioning methods, I: Self-adjoint and positive definite elliptic problems*, Numer. Lin. Alg. Appl., 1 (1994), pp. 75–101.

[4] T.J.R. Hughes, I. Levit, J.M. Winget, *An element-by-element solution algorithm for problems of structural and solid mechanics*, Comput. Meths. Appl. Mech. Engrg, 36 (1983), pp. 241–254.

[5] T.J.R. Hughes, J.M. Winget, *Solution algorithms for nonlinear transient heat conduction analysis employing element-by-element iterative strategies*, Comput. Meths. Appl. Mech. Engrg., 52 (1985), pp. 711–815.

[6] H. Yserentant, *On the Multilevel Splitting of Finite Element Spaces*, Numer. Math., 49 (1986), pp. 379–412.

Non-Conforming Triangular Finite Elements for the Wave Equation

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Finite element methods are convenient because they can handle arbitrary geometry and higher order methods are easy to construct. However, for the transient wave equation, they have the disadvantage that the "mass matrix" must be inverted at every time step, even if an explicit method is used. In order to avoid this inversion, one must mass-lump by putting the degrees of freedom at points of quadrature rules. This has been done easily for conventional quadrilateral and hexahedral finite elements by using products of Gauss-Lobatto 1D quadrature rules. For triangular and tetrahedral elements, one must add some degrees of freedom and use new quadrature rules. Moreover, it is difficult to handle complicated boundary conditions with these methods since the degrees of freedom of the trace of such elements do not correspond to the quadrature points of a sufficiently accurate quadrature rule.

In this talk, we discuss higher order non conforming triangular finite elements. We show that, in order to get best accuracy, one must choose degrees of freedom which fit with Gauss points on the edges of the triangles. This property enables us to deal easily with boundary conditions. We shall present error and dispersion analysis and numerical experiments to show the advantages and disadvantages of the new schemes. Extension to tetrahedral elements remains an open problem.

An Advanced Hybrid Numerical Solver for 3D Elastodynamics

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A. Quarteroni[‡§]

1 Introduction

The use of high order numerical methods has been recently proposed to simulate the propagation of elastic waves in solids with the aim of reducing computational effort and memory storage, or alternatively, to attain more accurate results in approximating smooth solution with the same number of nodes than in classical finite difference and finite element methods. On the other hand, finite elements allow a greater flexibility in dealing with problems posed on highly irregular domains or involving complex constitutive laws. It follows that numerical methods able to exploit the advantages of both approaches have a great potential for applications to realistic three-dimensional scenarios. In fact, geological media are in general inhomogeneous, irregularly shaped structures, and some parts of the soil may require non-linear models. Moreover, irregular surface topography should be taken into account to appropriately reproduce site effects, and seismic sources have to be included in the computational domain. In the present case, a hybrid spectral element - finite element algorithm has been developed, and it has been effectively implemented into a three-dimensional large capability code. The main idea is to use finite elements (FEM) in those portions of

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the computational domain where plastic behaviour, strong inhomogeneities or foundation interactions (in essence, non-linear phenomena) may occur. As a consequence, the medium in the complementary region has a linear visco-elastic behaviour and a smooth shape, allowing the use of a spectral element (SEM) discretization, which permits a strong reduction of the computational complexity and therefore possibility of extending the domain up to the source. A coupling algorithm based on the mortar projection method is then introduced for matching the solution on interfaces between different regions.

2 Problem formulation

Through the principle of virtual work, the dynamic equilibrium problem for a linear elastic solid in the presence of an external force distribution $\mathbf{f}$ can be stated in the following *weak*, or variational form (summation on repeated indices is assumed): *find* $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ *such that for each* $t \in (0, T)$ *and for each admissible displacement* $\mathbf{v}$*:*

$$\frac{\partial^2}{\partial t^2} \int_\Omega \rho \mathbf{u} \cdot \mathbf{v} d\Omega + \int_\Omega \sigma_{ij}(\mathbf{u}) \epsilon_{ij}(\mathbf{v}) \, d\Omega =$$

$$(1) \qquad \int_{\Gamma_N} \mathbf{t} \cdot \mathbf{v} \, d\Gamma + \int_{\Gamma_{NR}} \mathbf{t}^* \cdot \mathbf{v} \, d\Gamma + \int_\Omega \mathbf{f} \cdot \mathbf{v} \, d\Omega, \quad i, j = 1, 2, 3,$$

where t is the time, ρ the density and Ω the physical domain on which the problem (1) is defined with boundary $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_{NR}$. Γ_D is the portion in which the displacement vector $\mathbf{u}$ is prescribed, Γ_N the portion subject to external forces (tractions) $\mathbf{t}$, whilst on Γ_{NR} non reflecting boundary conditions are imposed by an appropriate choice of $\mathbf{t}^*$. Equations (1) should be supplemented with suitable initial conditions for both $\mathbf{u}$ and its time derivative. The stress and strain tensors in (1) are related to the displacement $\mathbf{u}$ by the Hooke's law

$$\sigma_{ij}(\mathbf{u}) = \lambda div \mathbf{u} \delta_{ij} + 2\mu \epsilon_{ij}(\mathbf{u}) \ , \quad \epsilon_{ij}(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad , \quad i, j = 1, 2, 3,$$

where λ and μ are the Lame's constants and δ_{ij} the Kronecker index.

3 Solution Algorithm

For the sake of clarity, we consider a simple computational domain Ω subdivided into two parts Ω^{fe} and Ω^{se}, with $\gamma := \partial\Omega^{fe} \cap \partial\Omega^{se}$ denoting the

common interface. In the FEM domain Ω^{fe}, the solution is approximated using piecewise polynomial functions N of low degree, whereas in the SEM computational domain Ω^{se} the solution is approximated by piecewise polynomial functions ψ of high degree defined onto hexahedra. Upon discretization of (1) the following expression for the semi-discrete equation of motion is obtained:

$$\tilde{m}\ddot{\mathbf{u}} = \mathbf{f}^{ext} - \mathbf{f}^{int} + \mathbf{r} \ ,$$

where $\tilde{m}$ is the mass matrix, $\mathbf{f}^{int}$ is the vector of nodal internal forces equivalent to the element's internal stress states, and $\mathbf{r}$ are the $n_{fe}+n_{se}$ unknown interaction forces at the interface γ. In order to make the problem consistent, we need to specify a relation between the FEM and the SEM solutions at the interface γ. The well known integral matching condition for elliptic problems, which is at the base of the *mortar* method has been extended to our wave propagation problem. This condition is written as follows:

$$\int_\gamma (\mathbf{u}^{fe} - \mathbf{u}^{se}) N_j' d\gamma = 0 \qquad j = 1, ..., n_{fe} \tag{2}$$

where N_j' are the n_{fe} FEM admissible displacements non vanishing on the interface or, in other words, the FEM basis functions centered on the n_{fe} finite element nodes lying on γ.
It can be demonstrated that the choice of condition (2) brings *optimal* accuracy, in the sense that the global approximation error turns out to be the sum of two independent contributions, one from the FEM, the other from the SEM. After time discretization, the solution is adavanced in time explicitly in both the FEM and SEM domains, while it requires the solution of a small algebraic problem for determining the solution at the interface.

4 Applications

The above presented hybrid method based on the mortar FEM/SEM approximation, is particularly well-suited for the numerical treatment of complex wave simulation problems involving highly heterogeneous media. In particular, the implementation of the coupling condition in terms of Lagrange multipliers results in a robust and general computational tool. Validation of the method on various test cases will be presented to demonstrate that the method enjoys the expected accuracy. The performance and capabilities of the proposed method are further assessed by considering examples

on realistic field-scale wave propagation scenarios. Finally, some new recent developments will be presented and discussed.

Boundary layers in thin plates

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This lecture addresses asymptotic expansions of displacement fields and strain tensors in thin elastic plates, and more specially the boundary layer part of them which is concentrated near the lateral boundary of the plates. The results which are presented rely on recent joint works with I. GRUAIS and A. RÖSSLE [1, 2] (mathematical approach of the asymptotics) and with Z. YOSIBASH [3] (computations with higher order methods).

We consider the displacement field solution u^ε of the linearized equations of elasticity in isotropic three-dimensional plates, with thickness 2ε and mean surface ω. The traction is imposed on the top and bottom surfaces $\omega \times \{\pm\varepsilon\}$. We consider different types of boundary conditions on the lateral surface $\partial\omega \times (-\varepsilon, \varepsilon)$: hard and soft clamped, hard and soft simply supported, free. In each situation we investigate the behavior of u^ε and of the corresponding strain tensor as $\varepsilon \to 0$.

Each asymptotics has two very different families of terms:

1) The outer expansion part which describe (in the in-plane variables and the scaled transverse variable) the global effects in the plate: this part includes e.g. Kirchhoff-Love displacements and the corresponding linear or quadratic transverse displacements which are associated with KL displacements.

2) The inner expansion part which describe (in a scaled distance to the lateral boundary and the scaled transverse variable) rapidly decreasing effects, which are strongly concentrated in a neighborhood of the lateral boundary (of width $\varepsilon \log \varepsilon$).

Each component of the displacement or of the strain has a different prevailings behavior according to
- the nature of lateral boundary conditions,
- the properties of the loadings (of stretching or bending type),
- the way it is investigated (pointwise values, localized mean values, etc...)
- the way it is computed (3D model, Reissner-Mindlin or hierarchical models).

We will present a few characteristic examples.

References

[1] M. DAUGE, I. GRUAIS, A. RÖSSLE. The influence of lateral boundary conditions on the asymptotics in thin elastic plates I: clamped and simply supported plates. Preprint 97-28, IRMAR, Université de Rennes I, Rennes 1997.

[2] M. DAUGE, I. GRUAIS, A. RÖSSLE. The influence of lateral boundary conditions on the asymptotics in thin elastic plates II: frictional, sliding edge and free plates. Preprint 97-29, IRMAR, Université de Rennes I, Rennes 1997.

[3] M. DAUGE, Z. YOSIBASH. Boundary layer realization in thin elastic 3-d domains and 2-d plate models. In preparation.

Sensitivity Analysis of Stress Intensity and Notch Factors in Elastic Structures

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Material discontinuities and geometrical peculiarities like cracks, notches, corners and edges lead to stress singularities in linear elastic structures. Their strength can be characterised by stress intensity or notch factors. These factors can be expressed as volume and surface integrals of given force densities and some non-energetic weight functions [1]. Their minimisation helps to avoid a damage of the elastic structure near interfaces, corner and edges. Here we investigate the influence of the shape of the domain and of the material parameters on the stress intensity and notch factors.
We proceed as follows using ideas of the material derivative approach [2,3,4]: We introduce a fixed reference configuration and regard a class of small perturbations of the domain or of the material parameters, respectively. The state equations as well as all quantities which are defined over the actual configuration are transformed to state equations and field quantities defined on the fixed reference configuration. Thus the investigation of shape and material parameter sensitivity reduces to the investigation of a regular perturbed boundary value problem for the transformed elastic fields. We expand the transformed quantities asymptotically with respect to the pertubation parameter and justify the asymptotics with the help of a–priori estimates in weighted Sobolev spaces. In this way we obtain existence and regularity results for the material derivatives of the displacement fields and of the weight functions and derive explicit formulas for the sensitivity of the stress intensity and notch factors.

References:

1. M. Bochniak, A.–M. Sändig, Computation of generalized stress intensity factors for bonded elastic structures. Bericht 97/41 des SFB 404, University Stuttgart, 1997
2. B. Palmerio, A. Dervieux, Hadamard's variational formula for a mixed problem and an application to a problem related to a Signorini–like variational inequality, Numer. Funct. Anal. Optim. 1 (1979) pp. 113–144
3. O. Pironneau, Optimal Shape Design for Elliptic Systems, Springer–Verlag, New York, 1984
4. J. Sokolowski, J.P. Zolesio, Introduction to Shape Optimization, Springer–Verlag, Berlin, 1992.

NUMERICAL ANALYSIS OF SINGULARITIES IN THREE-DIMENSIONAL ELASTICITY

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A numerical method is described for the computation of eigen-pairs which characterize the exact solution of linear elastostatic problems in three-dimensions in the vicinity of edge and vertex singularities. These may be caused by re-entrant corners, abrupt changes in boundary conditions or material properties.

Such singularities are of great interest from the point of view of failure initiation: The eigen-pairs characterize the straining modes and their amplitudes quantify the amount of energy residing in particular straining modes. For this reason, failure theories directly or indirectly involve the eigenpairs and their amplitudes.

The problem of determining the eigen-pairs numerically on the basis of the modified Steklov formulation (presented in [1]) in conjunction with the p-version of the finite element method is presented. The weak eigen-problem for determining eigen-pairs is formulated both for edge and vertex singularities.

For edge singularities, the edge is excluded from the domain over which the integral is computed, thus high-order finite element methods provide exponential convergence rates for the eigen-pairs. Numerical results are provided for several cases including isotropic as well as anisotropic multi-material interfaces.

For vertex singularities the weak eigen-problem is more complicated if edges intersect at the vertex. In this case although the vertex can be excluded from the integration domain, the edges have to be treated carefully when high-order FE methods are being applied because of the edge-singularities.

References

[1] Z. YOSIBASH. Numerical analysis of edge singularities in three-dimensional elasticity. *Int. Jour. Numer. Meth. Engrg.*, 40, (1997), pp. 4611-4632.

Simulation of the Taylor-Couette flow in an hourglass geometry by spectral elements

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1 Introduction

The purpose of the algorithm presented here is to simulate the flow in an axisymmetric geometry of quadrangular cross section, with no more than two curved facing borders, the others being kept straight and at right angle with the former countours. The operations' count necessary to solve the Navier-Stokes equations in such a domain is estimated as the triple of the cost necessary on a rectangular domain.

2 Simulations in a rectangular domain

We have compared our simulations to the experimental results of Andereck et al. [1]. As they observed, and as did G. I. Taylor before them, when only the inner cylinder is rotating, a transition occurs from the laminar Couette flow to a periodic superposition of vortices, called the Taylor vortex flow, as the velocity is increased. This transition should occur at a critical Reynolds number: $Re_c = 118.09$, for the case of infinitely long cylinders and for a radius ratio, $\eta = \frac{R_{in}}{R_{out}}$, of 0.875. The gap being of finite length in our case, we multiply this critical Reynolds number by the correction factor: $1 + \frac{1}{\Gamma^2}$, Γ being the aspect ratio of the rectangular cavity, to get the right value: $Re_c = 118.22$. The critical Reynolds number calculated by our code for this transition is: 118.24. This small discrepancy is due to the fact that we had to stop our time dependent calculation before the steady state was reached, because of the exponantially growing amount of time needed to obtain a more accurate solution. More puzzling, at first sight, is the non negligible difference between the wave number we have calculated: $\lambda = 3.07$, and the analytical one: $\lambda = 3.12$. This difference is due to the adaptation of the height of the Taylor vortices to fit the available vertical space. This is known as the quantization problem. The presence of the lower and upper walls imposes an even number of vortices. Each Ekman cell having a length of about 1.3 gap width, in the range of Reynolds numbers we are interested in, one finds easily that the number of vortices of correct length should be 27.6. The nearest even integer, 28, is chosen instead. The vortices then have to shorten a little as can be seen in figure 1.

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StreamRe130.ps

Figure 1: Streamlines showing a Taylor vortex a little above mid-height. $\Gamma = 30$, $\eta = 0.875$ and $Re = 130$.

3 Description of the algorithm in a curved quadrangular domain

The Navier-Stokes equations for an incompressible fluid are discretized using Fourier expansions in the periodic azimuthal direction and spectral elements in the (r, z) plane. We call:

- (r, z) the initial radial and axial coordinates in Ω,
- (x, y) the new radial and axial coordinates in the reference square $\hat{\Omega}$.

The spurious pressure modes are supressed by using a modified version of the (P^N/P^{N-2}) formulation, designed by Azaïez et al. [2], which uses the same grid for both pressure and velocity.
Time marching is performed via an explicit second order Runge-Kutta scheme. The time stepping is adaptive. The pressure is decoupled from the velocity by the solution of a pseudo-Laplacian on the pressure. Compared to a Laplacian that demands pressure boundary conditions, the pseudo-Poisson needs velocity boundary conditions.

The mapping chosen to transform the quadrangular domain, Ω, into the reference square, $\hat{\Omega} = [-1,1] \times [-1,1]$, is the first order transfinite interpolation of Gordon and Hall [3].
We assume that only two facing contours are deformed from the original reference square, $\hat{\Omega}$, in our case the two vertical cylinders, Γ_1 and Γ_3. The previous assumption implies that the axial direction, z, as well as the Jacobian of the transformation, J, depend only on y, while the radial direction, r, varies with both x and y. Without any loss of generality we may write $r(x,y)$ as: $a(x)b(y) + c(x)$, a, b and c being linear functions. In the general case where the four contours are curved, we would have a similar expression for $z(x,y)$ and $J(x,y)$. The geometrical simplification we introduced enables us to write the ordinary differential equations (ODE) resulting from the spatial discretization in tensor form. This would not be possible in the general case due to the appearance of $\frac{1}{J(x,y)}$ in the diffusive term. The tensorization would however still be possible if $J(x,y)$ were separable in the product of a function of x by a function of y. Let us call:

- K^r, the number of elements in the radial direction,
- K^z, the number of elements in the axial direction,
- N^r, the polynomial degree in the radial direction and
- N^z, the polynomial degree in the axial direction.

Though, the operation count of our algorithm: $3(K^r N^{r2} + K^z N^{z2})$ additions and multiplications, is three times that in a rectangular domain, it still is a lot smaller than in the general case where the ODEs are not tensorizable, and for which the operation count is: $\max(K^r, K^z)\,(\min(K^r, K^z)N$ additions and multiplications.

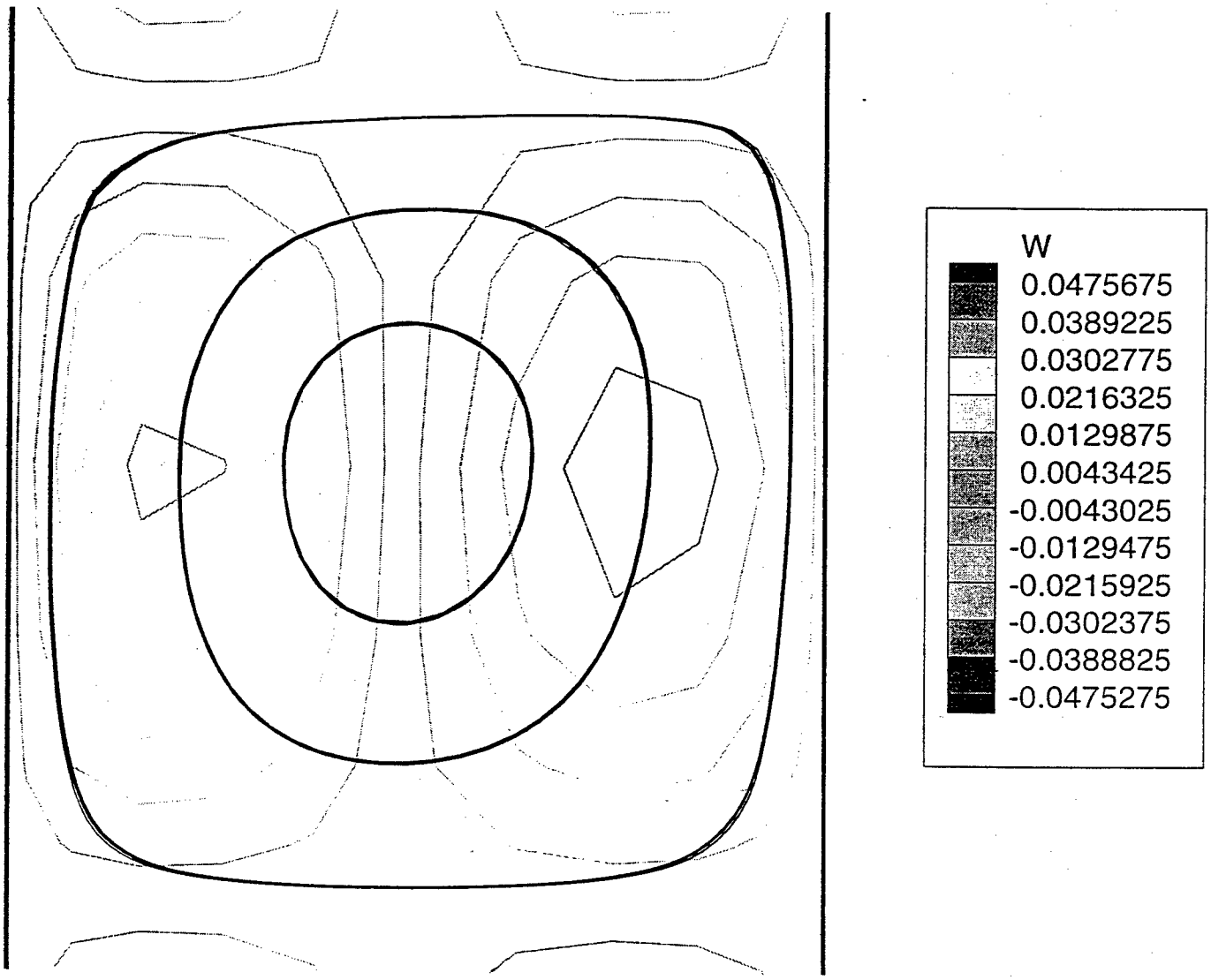
The validation of the corresponding program is in progress and the first results of simulation will be presented at the conference.

References

[1] C. D. Andereck, S. S. Liu and H. L. Swinney.
Flow regimes in a circular Couette system with independently rotating cylinders.
Journal of Fluid Mechanics 164 (1986).
Pages 155-183.

[2] M. Azaïez, A. Fikri and G. Labrosse.
A unique grid spectral solver of the nD Cartesian unsteady Stokes system. Illustrative numerical results.
Finite Elements in Analysis and Design 16 (1994).
Pages 247-260.

[3] W. J. Gordon and C. A. Hall.
Transfinite Element Methods: Blending-Function Interpolation over Arbitrary Curved Element Domains.
Numerische Mathematik 21 (1973).
Pages 109-129.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Efficient low-order preconditioning for fully-coupled and high-order finite volume Navier-Stokes solvers

ICO98-92

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Abstract –

An efficient fully-coupled solver based on high-order compact finite volume methods is constructed and validated on the incompressible Navier-Stokes equations. We write the 2-D set of unsteady equations under a conservative formulation in primitive variables. The system is discretized in time using a fourth-order backward linearly-implicit scheme in which nonlinear advective terms are linearized by extrapolating one of the multipliers. The space discretization is assured by a fourth-order compact finite volume method $CFV4$ [Kortas and Angot, 1997] [Kortas and Angot, 1998] built on a staggered mesh of type MAC. At each time step, the fully-coupled system for velocity and pressure unknowns is solved by preconditioned Krylov subspace methods: $BiCGSTAB(2)$ or $GMRESR$. The fourth-order accuracy in time and space is both achieved for velocity and pressure for instance on the analytical solution of the Green-Taylor vortex [Kortas, 1997].

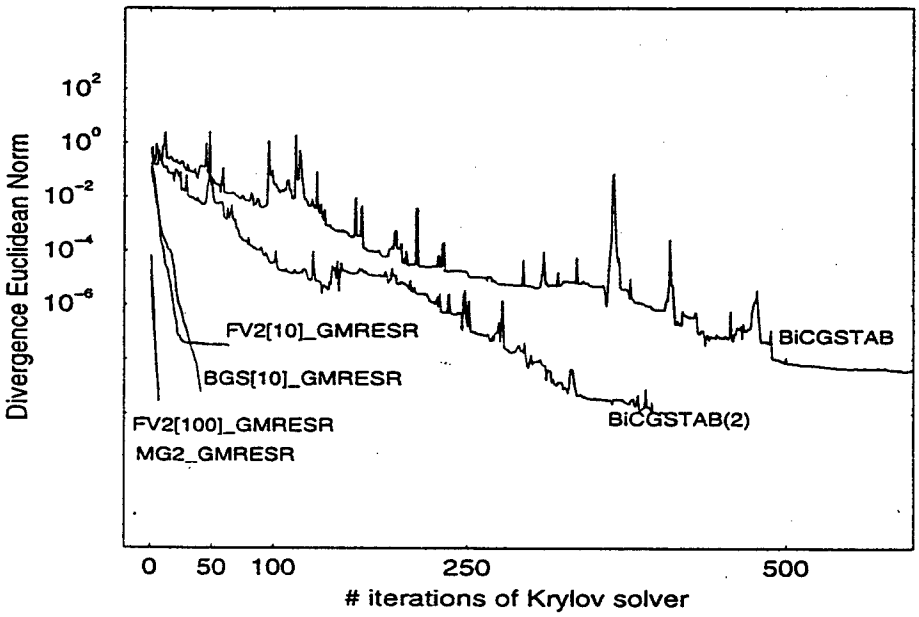

Figure 1: Convergence history for the Green-Taylor problem at $Re = 10$ on a 135×135 grid.

We compare several low-order preconditioners based on the finite volume second-order discretization $FV2$ of the same system of equations. It also includes first-order upwinding of the advective terms for better stability properties. The best results are obtained with $MG2\_CFV4$, i.e. for a multigrid solver $MG2$ [Vanka, 1986] used as preconditioner for $FV2$. The multigrid solver is based on a "cell by cell" Symmetric Block Gauss-Seidel BGS smoother, bilinear interpolation for prolongation and canonical restriction between successive grids with a mesh step ratio equal to 3.

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preconditioning is divided by 50 with the preconditioned solver $MG2\_CFV4$ (see Fig. 1). The condition number is thus divided by 2500 ! For example, this allows us to divide the computation time of $CFV4$ by 25 on a 81×81 grid. This improvement both comes from the efficiency of the low-order preconditioner $FV2$ and from the multigrid acceleration $MG2$.

On an IBM SP2 node, for the 135×135 grid, the computational cost of $MG2\_CFV4$ is only 1.7 times higher than for $MG2$, which is reputed to be very fast at least on a steady case problem [Vanka, 1986]. Hence with the reference grid of size 135×135 for $MG2$, we observe on Fig. 2 that: to reach the same accuracy of 10^{-6} $MG2\_CFV4$ is proven to be about 50 times faster than $MG2$; using the same CPU time, $MG2\_CFV4$ is 500 times more accurate than $MG2$. Besides, dividing the error by 10 requires the CPU time to be multiplied by 30 with $MG2$, against only by 3 with $MG2\_CFV4$.

The robustness of the method $MG2\_CFV4$ is also tested for convection-dominated flows. The problem of the lid-driven cavity with regularized boundary conditions is investigated up to Reynolds number $Re = 5000$.

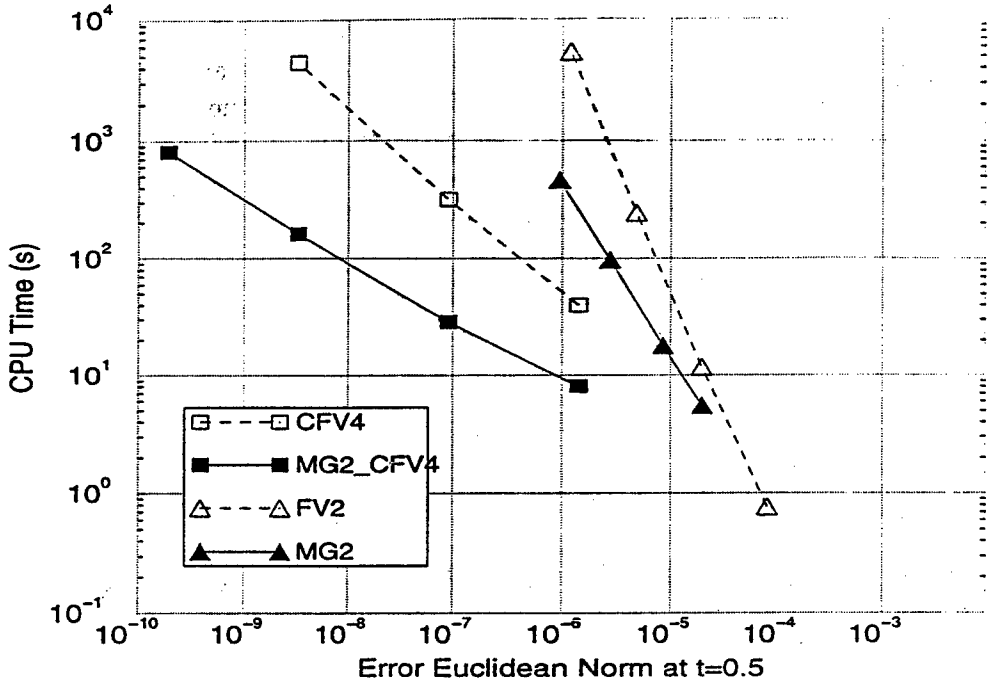

Figure 2: Comparison between $CFV4$ and $FV2$ for the Green-Taylor problem at $Re = 10$ and the same grid sizes: 27^2, 45^2, 81^2 and 135^2.

References

[Kortas, 1997] **S. Kortas,** *Préconditionnements multi-domaines et multi-niveaux de solveurs en volumes finis de haute précision; Implémentation sur machines parallèles*, Ph.D. Thesis in Appl. Math., Univ. Provence Aix-Marseille I, 22 sept. 1997.

[Kortas and Angot, 1997] **S. Kortas, Ph. Angot,** A New Class of High-Order Compact Finite Volume Schemes, Numer. Meth. for P.D.E.'s, 1997 (submitted).

[Kortas and Angot, 1998] **S. Kortas, Ph. Angot,** Parallel Preconditioners for a Fourth Order Discretization of the Viscous Bürgers Equation, in Proceedings 9th Int. Conf. on Domain Decomposition Methods for P.D.E., P. Björstad, M. Espedal and D. Keyes (Eds), J. Wiley & Sons, 1998.

[Vanka, 1986] **S.P. Vanka,** Block-implicit multigrid solution of Navier-Stokes equations in primitive variables, J. Comput. Phys., 65: 138-158, 1986.

A High Order Interface Capturing Technique for Structure Development in Binary Fluids

M. Verschueren, P.D. Anderson and F.N. van de Vosse

Introduction

The classical description of multi-phase flows with interfacial tension involves solving a moving boundary problem. Computationally, this approach is not very convenient in case of large interfacial deformations. To avoid this, surface tension may be incorporated using a locally acting volume force by the introduction of a "color function" which replaces the boundary conditions by a smooth density profile (Brackbill, 1991). Although reasonable results can be obtained using this method, the color function is not derived on basis of a physical model.

When the classical sharp interface is replaced by a small transition region, across which the thermodynamic variables change continuously, interfacial tension can be incorporated as a body force in the momentum equation. The shape and width of this transition region are not arbitrary. They are determined by the microscopic force balance at the interface. Since there are no rigorous theories available describing the processes at these small scales we follow the phenomenological Ginzburg-Landau approach [3,4], which includes spatial gradients of the order parameter in the Helmholtz free energy of the system. One of the advantages of this model is that it allows studying phenomena which cannot be described classically without the introduction of moving boundaries, such as Marangoni convection, break up, coalescence and phase separation. Full advantage of the accurate approximation of the steep gradients at the moving interface can be taken from high order methods, like the spectral element method applied in this study.

Method

A mean-field Ginzburg-Landau model (Cahn and Hilliard, 1958, Gunton et al., 1964) includes spatial gradients of the order parameter c in the Helmholtz free energy F of the system. For an isothermal binary fluid we have:

$$F[\rho, c, \nabla c] = \int_V (f_0(\rho, c) + \frac{1}{2}\epsilon(c)(\nabla c)^2)dV$$

where ϵ is a parameter related to the interfacial tension as:

$$\sigma = \epsilon \int_V (\nabla c)^2 dV$$

and f_0 is the homogeneous free energy density defined by:

$$f_0 = \frac{s}{4}c^4 - \frac{r}{2}c^2$$

r being a parameter proportional to temperature with respect to the critical temperature $(T_c - T)$ and $s > 0$. The non-classical chemical potential objective to c is:

$$\mu = \frac{\delta F}{\delta c} = \frac{\partial f_0}{\partial c} - \epsilon\nabla^2 c + \frac{1}{2}\frac{\partial \epsilon}{\partial c}(\nabla c)^2$$

Mass and momentum conservation can be written as

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \\ \rho \dfrac{\partial c}{\partial t} + \rho \vec{v} \cdot \nabla c = \nabla \cdot (\nu \nabla \mu) \\ \rho \dfrac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} = -\nabla p + \nabla \cdot \sigma + \mu \nabla c + \rho \vec{g} \end{cases}$$

The surface tension now is a locally acting volume force represented by $\mu\nabla c$. The term $\nabla \cdot (\nu \nabla \mu)$ in the composition equation allows for a continuous transition region between the two components of the system. In this way, like the color function, the density profile is continuous but now uniquely determined by the free energy of the system. A spectral element method, based on high order Legendre interpolation on Gauss-Lobatto integration points (Timmermans et al.,1994), is used to discretize the equations of motion and composition on a fixed grid.

Results and conclusion

A thermodynamically unstable region can be divided into two parts: a meta-stable region in which a finite perturbation is necessary to cause phase separation, and an unstable region in which every perturbation in unstable. Figure 1 shows the growth of a super-critical and decay of a sub-critical nucleus in a meta-stable surrounding (the top and bottom of the graph represent the equilibrium compositions).

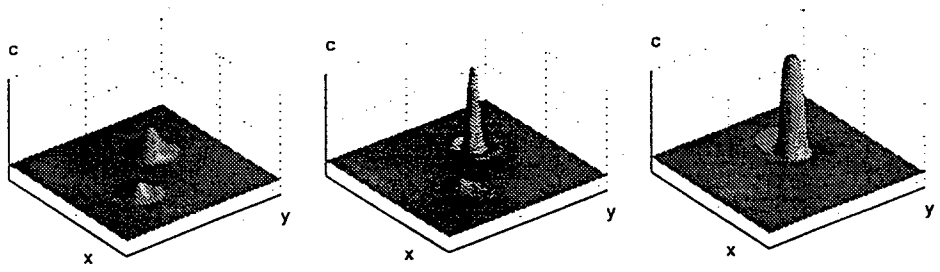

Figure 1: growth of a super-critical and decay of a sub-critical nucleus.

In problems as given above the concentration gradient of the nucleous, is essential for a proper simulation of the process and is very large. In table 1 both h and N convergence of ∇c is given showing the superior behaviour of the high order method.

Table 1: N- and h-convergence of ∇c at the interface.

	d.o.f = 8	d.o.f = 16	d.o.f=32	d.o.f=64
N = 2	0.3197	0.1673	0.0517	0.0213
N = 4	0.2344	0.1732	0.0122	0.0020
N = 8	0.2733	0.1177	0.0084	0.0007

Figure 2 shows the effect of interfacial tension gradients on a droplet (thick line). The interfacial tension is a monotonically increasing function of the y-coordinate. An initially arbitrarily shaped droplet becomes circular due to interfacial tension and moves downwards due to Marangoni convection.

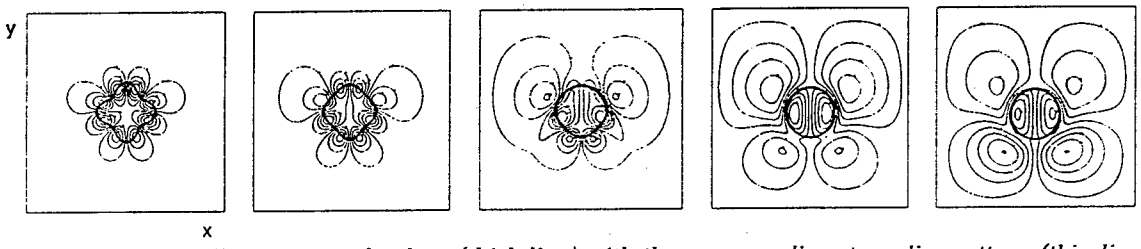

Figure 2: capillary motion of a drop (thick line) with the corresponding streamline pattern (thin lines).

The high accuracy and minimal diffusieve and dispersieve errors typical for spectral methods enable proper simulation of structure development in fluids by including a continuous change of thermodynamic variables at fluid-fluid interfaces.

References

1. J.U. Brackbill, D.B. Kothe and C. Zemach, A continuum model for modeling surface tension. *J. Comp. Phys.*, 100, 335-354 (1991).

2. J.W. Cahn and J.E. Hilliard, Free energy of a nonuniform system. I. Interfacial energy. *J. Chem. Phys.*, 28 (1958)

3. J.D. Gunton, M.S. Miguel and P.S. Sahni, *The dynamics of first-order phase transitions*, vol 8 of *Phase transitions and critical phenomena*, Academic Press, London (1964).

4. L.J.P. Timmermans, F.N. van de Vosse and P.D. Minev, Taylor-Galerkin based spectral element methods for convection-diffusion problems, *Int. J. Num. Meth. Fluids*, 18, 853-870, (1994).

Steady motion of a viscous fluid inside a circular boundary

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Numerical solutions are presented for steady two-dimensional motion within a circular cylinder generated by fluid injecting radially over one small arc and ejecting radially over another arc. These solutions are based on a mixed finite-difference pseudospectral method. Previous calculations were able to solve the problem for a range of Reynolds numbers from Re =0 to Re=20 only. The present results in this range of Reynolds number compare very well with those obtained by Mills (1977), Wang \& Wu (1986) and Dennis, Ng \& Nguyen (1993). The main object of this study is to extend the Reynolds number range for reliable solution, particularly with regard to the flow patterns, by using the spectral methods. Numerical solutions indicate that when Re is large these patterns are almost independent of the Reynolds number.

A Legendre Spectral Galerkin Method for the Biharmonic Dirichlet Problem

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Abstract

We consider a spectral Galerkin method for the biharmonic Dirichlet problem

$$\Delta^2 u = f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega,$$

where Δ denotes the Laplacian, $\Omega = (-1,1)\times(-1,1)$, $\partial\Omega$ is the boundary of Ω, and $\partial/\partial n$ is the outer normal derivative on $\partial\Omega$. Recently, efficient spectral Galerkin methods, which are based on the standard variational formulation of the problem, have been considered in [1], [2], and [3]. In this talk, following the approach of Ciarlet and Raviart, we introduce $v = \Delta u$ to obtain the coupled problem

$$-\Delta u + v = 0 \text{ in } \Omega, \quad -\Delta v = -f \text{ in } \Omega, \quad u = \partial u/\partial n = 0 \text{ on } \partial\Omega.$$

For a positive integer N, let P_N be the set of polynomials of degree $\leq N$ on $(-1,1)$, and let $P_N^0 = \{p \in P_N : p(\pm 1) = 0\}$. Let

$$X_N = \{w \in P_N \otimes P_N : w(\alpha,\beta) = 0, \alpha,\beta = -1,1\}, \quad X_N^0 = \{w \in P_N^0 \otimes P_N^0\}.$$

Our spectral Galerkin problem consists in finding $U \in X_N^0$ and $V \in X_N$ such that

$$\int_\Omega V\eta\, d\Omega + \int_\Omega \nabla U \cdot \nabla\eta\, d\Omega = 0, \quad \eta \in X_N,$$

$$\int_\Omega \nabla V \cdot \nabla\delta\, d\Omega = -\int_\Omega f\delta\, d\Omega, \quad \delta \in X_N^0.$$

We prove existence and uniqueness of the Galerkin solution and establish error bounds in Sobolev norms. The matrix-vector form of the spectral Galerkin problem is derived using the basis functions of [2] for the space

P_N^0; each basis function being a linear combination of two Legendre polynomials. We use a Schur complement approach to reduce the resulting linear system to a linear system involving the approximation V of v on the two vertical sides of $\partial\Omega$ and to an auxiliary Galerkin problem for a related biharmonic problem with v instead of $\partial u/\partial n$ specified on the two vertical sides of $\partial\Omega$. The Schur complement system with a symmetric and positive definite matrix is solved using the preconditioned conjugate gradient method. A preconditioner is obtained from the Galerkin problem for a related biharmonic problem with v instead of $\partial u/\partial n$ specified on the two horizontal sides of $\partial\Omega$. It is conjectured that the preconditioner is spectraly equivalent to the Schur complement matrix. The cost of solving a linear system with the preconditioner and the cost of multiplying the Schur complement matrix by a vector are $O(N^2)$ each. With the number of iterations proportional to $\log N$, the cost of solving the Schur complement system is $O(N^2 \log N)$. The solution to the auxiliary Galerkin problem is obtained at a cost $O(N^3)$ using separation of variables and the solution of two symmetric eigenvalue problems with tridiagonal matrices. Hence the total computational cost of solving the Galerkin problem is $O(N^3)$. Numerical results demonstrate the spectral accuracy of the method in the approximations for u and v.

[1] P.E Bjørstad and B.P. Tjøstheim, *Efficient algorithms for solving a fourth-order equation with the spectral-Galerkin method*, SIAM J. Sci. Comput., 18 (1997), 621–632.

[2] J. Shen, *Efficient spectral-Galerkin method I. Direct solvers of second- and forth-order equations using Legendre polynomials*, SIAM J. Sci. Comput., 15 (1994), 1489–1505.

[3] J. Shen, *Efficient spectral-Galerkin method II. Direct solvers of second- and forth-order equations using Chebyshev polynomials*, SIAM J. Sci. Comput., 16 (1995), 74–87.

Title:

An adaptive Wavelet ADI methods for Combustion Problems

ICO98-96

by Wei Cai

Abstract:

In this talk, we will extend our one dimensional wavelet collocation methods for initial boundary value problems of PDEs (SIAM J. NA,June, 1996)
to the case of two dimensional problems with an ADI factorization for efficient time marching. The spline wavelet is constructed for the Sobolev space $H^2(I)$ on a closed interval with additional boundary wavelets and scaling functions. The wavelet basis from these special wavelet functions forms a hierarchical basis over the proposed collocation points. As a result, a fast discrete wavelet interpolation transform between function values and wavelet interpolation expansion coefficients is achieved with O(n long n) complexity. The two dimensional
wavelet scheme coupled with ADI methods provides the advantage of both local mesh refinement of finite element methods and the efficient solver property of the traditional ADI methods. Numerical results for two

dimensional flame propagations will be presented.

Abstract of the talk:

Discontinuous Galerkin Finite Element Method for Hamilton-Jacobi Equations

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Consider the nonlinear Hamilton-Jacobi equations (HJ)

$$\frac{\partial \varphi}{\partial t} + H\left(\varphi_{x_1}, ..., \varphi_{x_n}\right) = 0, \quad \varphi\left(x, 0\right) = \varphi^0\left(x\right).$$

A widely applied class of numerical schemes for (HJ) is the class of finite difference schemes, which require a structured mesh and hence are difficult to apply to complicated geometry or for adaptive mesh refinements. First and second order finite volume schemes, based on arbitrarily triangulation, were developed by Abgrall (1996) and Lafon and Osher (1996). However, higher order finite volume schemes face the problem of reconstruction on arbitrary triangulation, which is quite complicated, according to Abgrall (1996).

It is known [Lions, 1982], that the viscosity solution of HJ is equivalent to the entropy solution of the weakly hyperbolic system of the conservation laws

$$\frac{\partial w_i}{\partial t} + \frac{\partial}{\partial x_i} H\left(\mathbf{w}\right) = 0, \quad w_i\left(x, 0\right) = w_i^0\left(x\right) = D\varphi^0\left(x\right).$$

where $w_i = \varphi_{x_i}$ a.e. in $W^{1,\infty}$, $i = 1, ..., n$. The Runge-Kutta discontinuous Galerkin method for the strongly hyperbolic systems of conservation laws was presented and analyzed in a series of papers by Cockburn and Shu (1989, 1997). We adapt this method to solve the Hamilton-Jacobi equations, recovering the partial derivatives of φ from polynomials approximating w at every time stage by the least square approximation.

The method can be designed for any order of accuracy in space and in time. It combines the flexibility of finite element method in the easy handling of complicated geometry with the high resolution property for discontinuous solutions of finite difference and finite volume methods through monotone fluxes or approximate Riemann solvers applied at the element interfaces and limiters. It is an explicit method, so no global linear or nonlinear system has to be solved, the method has a local compact stencil suited for efficient parallel implementation.

We prove the total variation stability of the method in the one dimensional case and the element average L^∞ stability for certain functions H in the multidimensional case ($H \in L^\infty$; $H = F \circ G$ where G is linear; $H\left(\mathbf{w}\right) = \sum H_i\left(w_i\right)$ and $\varphi^0\left(x\right) = \sum \psi_i\left(x_i\right)$). We also show that recovering $D\varphi$ from the approximation of w by the least square at each time stage does not increase the element average L^∞ norm or the L^2 norm of the approximate solution and that this procedure is necessary for the desired order of accuracy.

One and two dimensional numerical examples are given to illustrate the capabilities of the method.

A postprocess based improvement of the spectral element method

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Keywords: Dissipative equations, spectral element method.

In recent years the numerical solution of dissipative partial diferential equations has received an inflow of ideas from the theory of dynamical systems. An important contribution is the use of approximate inertial manifolds in the so-called nonlinear Galerkin methods [7]. One of the most often mentioned advantages of nonlinear Galerkin methods over classical Galerkin discretizations is their higher convergence rates [3].

In [6], based on results in [4], an inexpensive novel technique to increase the accuracy and computational efficiency of Fourier spectral methods was developed. This technique was extended in [5] to spectral polynomial approximations overcoming some of the shortcomings of the previous methods. In both cases the postprocess yields the same accuracy as a nonlinear Galerkin method, [3], [8], while the computational cost is kept nearly the same as standard Galerkin, so that the postprocessed Galerkin method is more efficient than both standard and nonlinear Galerkin discretizations; see [6], [5].

In this talk we introduce a postprocess of the spectral element method [1], [2] for time-dependent dissipative equations. Let Ω be a two dimensional domain with smooth boundary. We consider equations that can be written in the form:

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= \nu \Delta u(x,t) + R(u(x,t)) + f(x,t), \quad 0 \le t \le T, \quad x \in \Omega, \\ u(x,0) &= u_0(x), \quad x \in \Omega, \\ u(x,t) &= 0, \quad x \in \partial\Omega, \end{aligned} \tag{1}$$

where R can be a nonlinear convective term such as $R(u) = (u \cdot \nabla)u$, or a reaction type term such as $R(u) = g(u)$, for g a given smooth function. We will assume that the source term is smooth enough so as to guarantee that both, the solution u and its time-derivative u_t, belong to the Sobolev space $H^s(\Omega)$, $s > 3/2$, for all $0 \le t \le T$.

The new approach may be summarize as follows: Suppose that the approximation is wanted at time $T > 0$. We first compute the Galerkin approximation based on a space of piecewise polynomials of degree N by numerically integrating the equation in the time interval $[0, T]$. Then, we postprocess by solving at the final time T a discrete linear elliptic problem on a space of piecewise polynomials of degree $M > N$. The rate of convergence of the resulting method is proved to be $\min(N^{-s-1}, M^{-s})$, so that, the method possesses a higher rate of convergence than the Galerkin method upon which the postprocess is applied. Since the elliptic problem in the higher order polynomial space is solved only

once, when the time integration is completed, the overcost of the postprocessed procedure is nearly negligible. Numerical experiments showing the superiority of the new method are presented.

References

[1] C. Bernardi and Y. Maday, *Approximation results for spectral methods with domain decomposition*, Appl. Numer. Math., 6 (1989/90), pp. 33-52.

[2] C. Canuto, M.Y. Hussaini, A. Quarteroni and T.A. Zang, Spectral methods in fluid dynamics, Springer Series in Computational Mathematics, Springer-Verlag, Berlin, 1988.

[3] C. Devulder, M. Marion and E.S. Titi, *On the rate of convergence of Nonlinear Galerkin method*, Math. Comput., 60 (1993), pp. 495-514.

[4] C. Foias, O. Manley and R. Temam, *Modelling of the interaction of small and large eddies in two dimensional turbulent flows*, RAIRO M^2AN, 22 (1988), pp. 93-114.

[5] J. de Frutos, B. García-Archilla and J. Novo, *A popstprocessed Galerkin method with Chebyshev or Legendre polynomials*, Applied Mathematics and Computations Reports, U. Valladolid, July 1996.

[6] B. García-Archilla, J. Novo and E.S. Titi, *Postprocessing the Galerkin method: A novel approach to Approximate inertial manifolds*, SIAM J. Numer.Anal., to appear.

[7] M. Marion and R. Temam, *Nonlinear Galerkin methods*, SIAM J. Numer. Anal., 26 (1989), pp. 1139-1157.

[8] J. Shen and R. Temam, *Nonlinear Galerkin method using Cehbyshev and Legendre polynomials I. The one-dimensional case.* SIAM J. Numer. Anal., 32 (1995), pp. 215-234.

Difference Potentials

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Abstract

In this talk, we provide a concise survey of the key ideas, apparatus, and applications of the difference potentials method (DPM). Among the issues to be discussed are:

- A construction of difference potentials for solutions of the general systems of linear difference equations that is analogous to the Cauchy-type integrals for solutions of the Cauchy-Riemann system (analytical functions).
- Modification of the Calderon-Seeley pseudodifferential boundary equations proposed by the author and the DPM as a methodology to use these modified equations for the numerical solution of internal and external boundary value problems.
- The DPM-based approach to setting the artificial boundary conditions.
- The DPM-based model of an active shielding problem and a general formula for all active shielding control functions.

References

1. V. S. Ryaben'kii, *Difference Potentials Method for Some Problems of Continuous Media Mechanics*, Nauka, Moscow, 1987 (Russian).
2. V. S. Ryaben'kii, *An Introduction to Numerical Mathematics*, Nauka, Moscow, 1994 (Russian).
3. V. S. Ryaben'kii, *Boundary Equations with Projections.* Russian Mathematical Surveys, Vol. 40 No. 2 (1985) pp. 147–183.
4. V. S. Ryaben'kii, *Difference Potentials and Their Applications*, ICASE Report No. 97-489, 1997.

Stratification of Matrix Spectra and the Problem of More Precise Statements of Standard Spectral Problems

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Abstract

The lecture is devoted to a survey of paradox situations that arise in the use of standard algorithms and programs (like MATLAB) for spectral problems of linear algebra. The reason of such paradoxes is that the statements of problems are ill-posed from the viewpoint of calculus. For example, the result of the work of some algorithm may contain insufficient information about the accuracy of the result and about the accuracy of data of the problem that is required for the needed accuracy of the result we want to obtain. In the author's opinion, the development of well-posed problems is of great importance for creating good computer procedures. In particular, this question was discussed by the author and his colleagues in [1–6].

For computation of the full collection of eigenvalues a number of versions of the QR algorithm was developed, and many of these versions work successfully. However, applying them to matrices with spectral clusters or even large spots of the ε-spectrum (the so-called spectral spots) sometimes leads to the results that look like dead ends.

The author suggests several statements of problems of the annular or linear (by straight lines parallel to the imaginary axis) stratification of the spectra. Bases for invariants subspaces are determined and some criteria for the dichotomy parameters are also indicated. The dichotomy parameters characterize the distance between clusters as well as the angle between the invariant subspaces that correspond to these clusters. To clarify the linear dichotomy it is convenient to replace this problem by the problem of the elliptic dichotomy.

It is likely that the creation of modified version of the QR algorithm designed for obtaining some of the above-mentioned spectral stratifications is not a difficult problem since similar algorithms could be composed from pieces of the well-known and widely used algorithms. Using such modifications of the QR algorithm, we obtain block-triangular matrices whose diagonal blocks are ordered in a certain way. After that we could study these matrices in order to find the dichotomy parameters corresponding to different blocks of the matrices.

The creation of spectral portraits proposed by the author and Prof. Trefethen is often very elaborate. The author now suggests a simplified scheme of graphical representation of the results obtained with some modified QR algorithms, the so-called schematic spectral portraits, which could be convenient for engineering.

The solvability of problems of spectral stratification requires the existence of such a stratification. In the study of this question, some ideas of M.V. Keldysh can be very useful.

In particular, M.V.Keldysh had suggested the characterization of the classes of matrices that admit such a stratification which can be obtained through the powers of singular values. These questions were discussed in the framework of the operator theory by Keldysh and Lidskii (see, for example, [7]).

References

1. S. K. GODUNOV, *Problems of guaranteed accuracy in numerical methods of linear algebra*, Proceedings of the International Congress of Mathematicians, 1986, August 3–11, 1986, Berkeley, California, Vol.2 (1986) pp. 1353–1361.

2. S. K. GODUNOV, V. I. KOSTIN, AND A. D. MITCHENKO, *Computation of an eigenvector of a symmetric tridiagonal matrix,* Sibirsk. Mat. Zh., Vol. 26, No. 5 (1985) pp. 71–85 (Russian); Siberian Math. J., Vol. 26 No. 5 (1985) pp. 684–695.

3. S. K. GODUNOV AND S. V. KUZNETSOV, *Estimates for convergences of the orthogonal-power method,* Trudy Inst. Mat. Sibirsk. Otdel. Ross. Akad. Nauk, Vol. 26 (1994) pp. 20–41 (Russian); Siberian Advances in Math., Vol. 5 No. 1 (1995) pp. 16-41.

4. S. K. GODUNOV, A. G. ANTONOV, O. P. KIRILYUK, AND V. I. KOSTIN, *Guaranteed accuracy for solutions of system of linear equations in Euclidean spaces,* Nauka, Novosibirsk, 1988 (Russian); Kluwer Academic Publishers, Dordrecht, 1993.

5. A. YA. BULGAKOV, *An effectively calculable parameter for the stability property of a system of linear differential equations with constant coefficients,* Sibirsk. Mat. Zh., Vol. 21, No. 3 (1980) pp. 32–41 (Russian); Siberian Math. J., Vol. 21 (1980) pp. 339–346.

6. S. K. GODUNOV, *Modern Aspects of Linear Algebra,* Nauchnaya Kniga, Novosibirsk, 1997 (Russian); AMS Series: Translations of Mathematical Monographs, Vol. 175.

7. M. V. KELDYSH AND V. B. LIDSKII, *Issues in Spectral Theory of Non-Self-Adjoint Operators*, in Proceedings of the Fourth Soviet National Congress of Mathematicians, Vol. 1, 1963, pp. 101-120.

An Approach to the Derivation of the Difference Potentials

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Abstract

It is shown that an accurate discrete implementation of the Calderon-Seeley construction of boundary potentials naturally leads to the difference potentials in the form of Reznik. Therewith, the result of Reznik is generalized for the case of a wide class of difference operators on non-regular (abstract) meshes with some natural restrictions on the structure of stencils.

Stable Difference Schemes for Parabolic Systems — A Numerical Radius Approach

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Abstract

In this talk we take a numerical radius approach in order to discuss sufficient stability conditions for a well-known family of finite difference schemes for the initial value problem associated with the Petrowski well-posed, multispace-dimensional parabolic system

$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \sum_{1\le p\le q\le s} A_{pq}\frac{\partial^2 \mathbf{u}(\mathbf{x},t)}{\partial x_p \partial x_q} + \sum_{1\le p\le s} B_p \frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial x_p} + C\mathbf{u}(\mathbf{x},t),$$

where A_{pq}, B_p and C are constant matrices, A_{pq} being Hermitian.

A Locally Implicit Second Order Accurate Difference Scheme for Solving Two-Dimensional Time-Dependent Hyperbolic Systems and Euler's Equations

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Abstract

A new difference method for solving two-dimensional time-dependent hyperbolic systems and Euler's equations is presented. This method is based on a unique difference scheme. The scheme is upwind quasi-monotone and provides second order accuracy in both space and time. The proposed scheme becomes implicit if and only if the corresponding Courant number is greater than one. It should be noted that typically the scheme is implicit with respect to some variables and it explicit with respect to the others. The method is aimed at solving the problems that involve the high aspect ratio cells. Efficiency of the scheme is demonstrated by the numerical results.

A Fast High Order Domain Decomposition Poisson Solver

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Abstract

We present a fast high order Poisson solver for implementation on parallel computers. The method uses deferred correction, such that high order accuracy is obtained by solving a sequence of systems with a narrow stencil on the left hand side. These systems are solved by a domain decomposition method. The method is direct in the sense that for any given order of accuracy, the number of arithmetic operations is fixed. Numerical experiments show that these high order solvers easily outperform standard second order ones. The very fast algorithm in combination with the coarser grid allowed for by the high order method, also makes it quite possible to compete with adaptive methods and irregular grids for problems with solutions containing widely different scales.

Parallel Solution of Helmholtz Problems using Additive Schwarz Methods

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Abstract

We demonstrate the use of additive Schwarz preconditioners in the solution of large-scale Helmholtz problems. Overlapping Schwarz methods with Sommerfeld-type conditions on the artificially introduced subdomain boundaries provide a practical degree of locality and concurrency. In conjunction with a Krylov method appropriate for complex-valued problems, good scalability is achieved for harmonic phenomena that are reasonably resolved with second-order discretizations. Generalizing the usual Dirichlet Schwarz interface conditions, such Sommerfeld-type boundary conditions avoid the possibility of resonant modes in the subdomains.

We present parallel performance results for model interior and exterior Helmholtz problems. For the latter we use so-called "exact" nonreflecting boundary conditions based on the Dirichlet-to-Neumann operator on the outer boundary. The PDE is discretized using finite elements and is enforced at all interior points. We emphasize that the subdomain problems with Sommerfeld-type conditions are used only in the preconditioner. Our implementation uses the Portable Extensible Toolkit for Scientific Computation (PETSc).

Difference Potentials for the Helmholtz Equation on Exterior Domains

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Abstract

Finite-difference methods are widely used for numerical solving boundary-value problems. In case the problem formulation permits to separate variables, efficient algorithms can be derived for corresponding discrete equations. However the method of separation of variables works usually only in problems having a "right" geometry like as parallelepiped, cylinder, sphere etc. At the same time, the *difference potentials method* (DPM) permits to generate fast equally efficient algorithms also for "non-right" geometry since it can explore separation of variables whenever the structure of governing differential equations admits to do this unlike both geometry and boundary conditions.

In the paper, we describe an algorithm for solving scattering problems governed by the Helmholtz equation:

$$\Delta u + \mu^2 u = 0 \quad \text{in } \mathbb{R}^3 \setminus D \tag{1}$$

$$lu \equiv \alpha u + \beta \frac{\partial u}{\partial n} = f \quad \text{on } \Gamma = \partial D \tag{2}$$

$$i\mu u + \frac{\partial u}{\partial r} = o(\frac{1}{r}) \tag{3}$$

where Δ is the Laplacian, μ is a positive constant, l is an operator of boundary conditions. Note that the algorithm has been developed in the early of eighteens; we present here an extended version of preprint [1].

Construction of proposed solution method consists of three basic stages described shortly below.

At first we discretize the Helmholtz equation (1) by using a central difference scheme in spherical coordinates. The difference scheme is considered inside a sphere, see Fig. 1, which is an artificial boundary. To treat the radiation condition (3) on S, we represent the solution outside the sphere by the Fourier series and use corresponding decay conditions separately for each radial Fourier coefficient. As a result, our difference scheme contains a non-local condition on the external boundary. Note that such type of the radiation condition is well-known and sometimes called *Dirichlet-to-Neumann* condition, see reviews [2], [3].

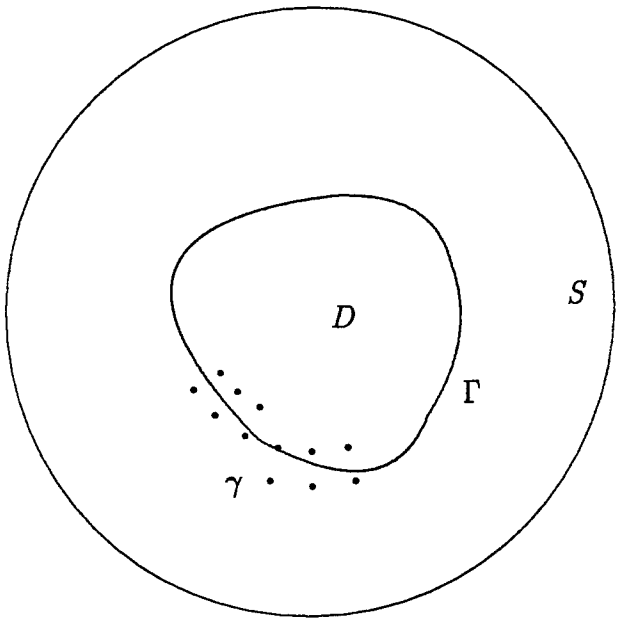

Figure 1: The artificial boundary (sphere) S and a portion of the mesh boundary γ

Then we reduce the difference governing equations from the mesh domain to *difference boundary equations* on the two-layer *mesh boundary*. This mesh boundary γ consists of mesh points belonging to cells that are intersected by the surface Γ, see Fig. 1 where several points of γ are shown. This reduction is made in accordance to the general scheme of DPM, see [4] and the paper by Ryaben'kii in the proceedings. The corresponding boundary equation has the form

$$Pu_\gamma \;=\; u_\gamma \tag{4}$$

where u_γ is a mesh function on γ, P is the difference potential operator. An important property of this reduction, especially as to the Helmholtz equation, is that the boundary equations are equivalent to the equations in the domain. Therefore our boundary equations are well-posed for all frequencies including those of internal resonances in D. The calculation of Pu_γ consists mainly of the solution of a difference problem posed in the "right" domain – between the sphere S and a small sphere inside D (not shown in Fig. 1) – and uses separation of variables.

Finally we formulate a discrete variational problem. To do this, we introduce a mesh of boundary elements on Γ with unknown Cauchy data $u_\Gamma = (u, \frac{\partial u}{\partial n})$ in nodes (third and second order formulae on elements are used to reconstruct u and $\frac{\partial u}{\partial n}$, respectively); introduce an operator Π that prolongs Cauchy data from Γ into the points of γ by the Taylor formula; introduce Euclidean spaces U_Γ of unknowns u_Γ and U_γ of mesh functions on γ equipped with norms $\|\cdot\|_\Gamma$ and $\|\cdot\|_\gamma$, respectively (the norms are chosen so that the resulting matrix is well-conditioned). The variational problem has the form: *find* $u_\Gamma \in U_\Gamma$ *such that*

$$\|P\Pi u_\Gamma - \Pi u_\Gamma\|_\gamma^2 + \|lu_\Gamma - f_\Gamma\|_\Gamma^2 \longrightarrow \min_{u_\Gamma \in U_\Gamma} \tag{5}$$

where $f_\Gamma = (f, 0)$ if $\alpha \neq 0$, and $f_\Gamma = (0, f)$ otherwise. Problem (5) is solved by using the conjugate gradients method (CGM).

The algorithm described above has the second order of approximation for smooth Γ and u. Numerical tests for bodies of revolution demonstrate the high accuracy of the method and rapid convergence of CGM iterations.

In the paper, we shortly describe also the technique of *difference spherical functions* [5] that are used in this and other algorithms.

Note that ideas of treating radiation conditions for this problem have been a starting point of research on generating exact boundary conditions in other problems: Maxwell equations [6], wave equation [7], linearized Navier-Stokes equation [8], linearized Euler equations [9].

References

[1] RYABEN'KII, V. S. & SOFRONOV, I. L. *A numerical solution of external spatial problems for the Helmholtz equation using the method of difference projectors.* Preprint No. 11, Keldysh Institute of Applied Mathematics, USSR Academy of Sciences, 1984 (in Russian).

[2] GIVOLI, D. Non-reflecting boundary conditions. *J. Comp. Phys.* **94**, 1–29 (1991).

[3] TSYNKOV, S. V. Numerical solution of problems on unbounded domains. A review. *Appl. Numer. Math.*, to appear.

[4] RYABEN'KII, V. S. *Difference potentials method for some problems of continuous media mechanics.* Moscow, Nauka, 1987 (in Russian).

[5] RYABEN'KII, V. S. & SOFRONOV, I. L. *Difference spherical functions.* Preprint No. 75, Keldysh Institute of Applied Mathematics, USSR Academy of Sciences, 1983 (in Russian).

[6] SOFRONOV, I. L. Difference potentials method for scattering problems described by the Maxwell equations, *Comput. Mech. of Solids*, Issue 2, 158–177, 1990 (in Russian).

[7] SOFRONOV, I. L. Conditions for complete transparency on the sphere for the three-dimensional wave equation. *Russian Acad. Sci. Dokl. Math.* **46**, 397–401 (1993).

[8] RYABEN'KII, V. S. & TSYNKOV, S. V. Artificial boundary conditions for the numerical solution of external viscous flow problems, *SIAM J. Numer. Anal.*, **32**, 1355–1389 (1995).

[9] SOFRONOV, I. L. Non-reflecting inflow and outflow in a wind tunnel for transonic time-accurate simulation. *J. Math. Anal. Appl.*, **221**, 92–115 (1998).

A Fast High Order Domain Decomposition Poisson Solver

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Abstract

Prandtl proposed the vortex sheet as an asymptotic model for a free shear layer in the zero viscosity limit. However, progress in understanding vortex sheet motion came slowly. The initial value problem is ill-posed in the sense of Hadamard, due to Kelvin-Helmholtz instability. It is known that analytic solutions exist locally in time, but Moore showed that a branch point singularity can form in the shape of an evolving vortex sheet. Computations using Chorin's vortex-blob method indicate that past the singularity formation time, the sheet rolls up into a spiral.

In this talk, I will discuss these issues and present recent work indicating the onset of chaos in vortex sheet roll-up. The initial data corresponds to potential flow past either a flat plate or a circular disk. The sheet rolls up into a vortex pair in the former (planar) case, and a vortex ring in the latter (axisymmetric) case. At early times, the roll-up proceeds smoothly. The flow enters a quasisteady state in which the core of the pair/ring undergoes small amplitude oscillations. At late times, the vortex sheet develops irregular small-scale features. The spiral turns in the core become nonuniformly spaced, and a wake is shed behind the vortex ring. These features are due to chaotic dynamics in the vortex sheet flow. The features in the core result from a *resonance* and the wake is due to a *heteroclinic tangle*. A Poincaré section shows that the vortex sheet flow resembles a periodically perturbed integrable Hamiltonian system, although chaos here is induced by self-sustained oscillations rather than external forcing.

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Issues in Constructing Absorbing Layers for Systems of PDE's

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Abstract

A detailed mathematical analysis of the Berenger PML method for the Electro-magnetic equations is carried out on the P.D.E. level, as well as for the semi-discrete and fully discrete formulations.

It is shown that the split set of equations is not strongly well-posed and that under certain conditions its solutions may be inappropriate.

A recently introduced system of partial differential equations, based on physical considerations, which describes the behavior of electro-magnetic waves in artificial absorbing layers, is analyzed. Analytic solutions are found, for the cases of semi-infinite layers and finite depth layers, both for primitive and characteristic boundary conditions.

A different set of equations that seem to offer some advantages is proposed in this paper. The properties of its solutions for the same geometries and boundary condition are also discussed. The methodology of constructing the new set of equation is based on mathematical rather than physical considerations. Therefore it can be also applied a to wave phenomena other than electromagnetics. We will show an application to advective acoustics.

Reflectionless Sponge Layers as ABCs for the Numerical Solution of Maxwell's Equations in Rectangular, Cylindrical, and Spherical Coordinates

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Abstract

A scaling argument will be used to derive reflectionless wave absorbing layers for the numerical solution of the elliptic and hyperbolic Maxwell equations in 3D rectangular, cylindrical and spherical coordinates. I will prove the reflectionless property in the elliptic formulation in all coordinate systems and show that the thusly obtained absorbing layers are described in the time-domain by causal, strongly well-posed hyperbolic systems. Also, I will analyze the numerical reflection of the discrete layers in cylindrical and spherical coordinates by calculating the numerical wavenumber of the discrete wave equation. This is made possible by employing appropriate addition theorems to calculate the action of the forward/backward shift operator on cylindrical and spherical Hankel functions, and on the spherical harmonics.

Numerical results will be given for scattering by cylinders and spheres in two and three dimensions, along with a comparison of the performance of the spherical sponge layer to that of the exact ABC derived by Grote and Keller for the 3D Maxwell's equations in spherical coordinates.

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Absolutely Transparent Boundary Conditions for Time-Dependent Wave-Type Problems[2]

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Abstract

A rigorous formulation of the artificial boundary conditions (ABCs) for the wave equation is presented. The exact nonlocal ABCs are obtained by means of the Riemann method. The corresponding Riemann function is used to formulate the exact ABCs for each Fourier mode. A sequence of approximate ABCs of different orders is presented as well. The first-order ABCs coincide with the well-known boundary conditions of Engquist & Majda (1977) and Tam (1993). The second order ABCs provide more accurate solutions. Comparison of the exact solution with both the first- and second-order numerical approximations corroborates the advantages of the second-order ABCs. The case of inseparable variables is included in the analyses.

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